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(54) Title: MUTANT PROTEINS, HIGH POTENCY INHIBITORY ANTIBODIES AND FIMCH CRYSTAL STRUCTURE

(57) Abstract: The present invention provides bacterial immunogenic agents for administration to humans and non-human animals to stimulate an immune response. It particularly relates to the vaccination of mammalian species, especially human patients, with variants of the *E. coli* FimCH protein that elicit antibodies that have better functional inhibitory activity than antibodies raised against wild type protein. In particular, such variants include mutations that promote a more open conformation of the FimH protein, particularly in regions involved in mannose binding, to expose regions previously poorly exposed and mutations that abolish a significantly reduce mannose binding. In another aspect, the invention provides antibodies against such proteins and protein complexes that may be used in passive immunization to protect or treat pathogenic bacterial infections. The present invention also provides machine readable media embedded with the three-dimensional atomic structure coordinates of FimCH bound to mannose, and subsets thereof, and methods of using the crystal structure to provide candidate amino acid residues for mutation.

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**MUTANT PROTEINS, HIGH POTENCY INHIBITORY ANTIBODIES  
AND FIMCH CRYSTAL STRUCTURE**

This application claims priority to U.S. Provisional Patent Application No. 60/254,353, filed December 8, 2000, and U.S. Provisional Patent Application No. 60/301,878, filed June 29, 2001, the content of each of which is incorporated herein by reference in its entirety.

**1. FIELD OF THE INVENTION**

The invention relates to methods of producing antibodies, preferably antibodies that inhibit binding of a protein to its binding partner. Further, the methods include producing antibodies having enhanced functional inhibitory activity against a protein, for example, that inhibit binding of the protein to a binding partner, by immunizing with a mutant form of the protein that elicits antibodies with greater inhibitory activity than those antibodies elicited by the wild type protein. In one example, mutant proteins are designed using the crystal structure of purified FimCH bound to mannose. Mutant proteins are expressed and used as antigens to elicit antibodies. Thus, this crystal structure, including its coordinates, and methods of designing vaccines and antibodies using information from the crystal structure are included herein. In particular embodiments, this invention relates to mutant bacterial adhesin proteins and active fragments thereof for use in the prevention, diagnosis and treatment of bacterial induced diseases such as those of the urinary tract. The invention encompasses use of mutant proteins as immunogenic agents in vaccine compositions to stimulate an immune response in humans and animals. The invention also encompasses the administration of antibodies to said mutant proteins to humans and animals in an effective amount, to treat, prevent or manage disease or infection. More specifically, the invention relates to the administration of purified mutant adhesin proteins or antibodies directed against said mutant adhesin proteins to a mammalian species as a mechanism to protect the vaccine or antibody recipient against infection by pathogenic bacterial species, including all types of Enterobacteriaceae.

**2. BACKGROUND OF THE INVENTION**

Urinary tract infections (herein, "UTI") present a disease process that is mediated (or assisted or otherwise induced) by the attachment of bacteria to cells. *Escherichia coli* is the most common pathogen of the urinary tract, accounting for more than



85% of cases of asymptomatic bacteriuria, acute cystitis and acute pyelonephritis, as well as greater than 60% of recurrent cystitis, and at least 35% of recurrent pyelonephritis infections. Furthermore, approximately 25%-30% of women experience a recurrent *E. coli* urinary tract infection within the first 12 months following an initial infection but after a second or third infection the rate of recurrence increases to 60%-75%. Given the high incidence, continued persistence, and significant expense associated with *E. coli* UTI, there is a need for a prophylactic treatment to reduce susceptibility to this disease.

Despite the overall prevalence of UTI in women, there have been few efforts to apply novel strategies in order to treat and/or prevent these diseases. Commonly, conventional antibiotics are used to treat these infections, such as treatment with penicillins, cephalosporins, aminoglycosides, sulfonamides and tetracyclines; in the special case of UTI, urinary antiseptics such as nitrofurantoin and nalidixic acid are employed, too. However, emerging antibiotic resistance will in the future hamper the ability to successfully treat UTI. Multiple antibiotic resistance among these uropathogens is increasing.

While many factors contribute to the acquisition and progression of *E. coli* UTI, it is generally accepted that colonization of the urinary epithelium is a required step in the infection process. In a typical course of *E. coli* urinary tract infection, bacteria originate from the bowel, ascend into the bladder, and adhere to the bladder mucosa where they multiply and establish an infection (cystitis) before ascending into the ureters and kidneys. Disruption or prevention of pilus-mediated attachment of *E. coli* to urinary epithelia may prevent or retard the development of UTI. In this regard, a number of studies have pointed to a role for pili in mediating attachment to host uroepithelial cells.

The initiation and persistence of many bacterial infections such as those described above is thought to require the presentation of adhesins on the surface of the microbe in accessible configurations which promote binding events that dictate whether extracellular colonization, internalization or other cellular responses will occur. Adhesins are often components of the long, thin, filamentous, heteropolymeric protein appendages known as pili, fimbriae, or fibrillae (these three terms will be used interchangeably herein). The bacterial attachment event is often the result of a stereo-chemical fit between an adhesin frequently located at the pilus tip and specific receptor architectures on host cells, often comprising carbohydrate structures in membrane associated glycoconjugates.

Uropathogenic strains of *E. coli* express P and type 1 pili that bind to receptors present in uroepithelial cells. The adhesin present at the tip of the P pilus, PapG, binds to the Gal $\alpha$ (1-4)Gal moiety present in the globoseries of glycolipids. Alternatively, the type 1 adhesin, FimH, binds D-mannose present in glycolipids and glycoproteins. Type



1 pili are thought to be important in initiating colonization of the bladder and inducing cystitis, whereas P pili are thought to play a role in ascending infections and the ensuing pyelonephritis.

5 With regard to type 1 pili, tip adhesins and other ancillary subunits also have been identified. FimH is the D-mannose-binding adhesin that promotes attachment of type 1 piliated bacteria to host cells via mannose-containing glycoproteins on eukaryotic cell surfaces. FimC is its periplasmic chaperone protein. It has recently been reported that such chaperones can direct formation of the appropriate native structure of the corresponding  
10 domain or helical strand of the chaperone or pilin. Thus, FimH proteins tend to have their native structure in the presence of such a chaperone but not in its absence (Choudhury *et al.*, 1999, *Science* 285:1061; Sauer *et al.*, 1999, *Science* 285:1058). In addition, recent publications have indicated that the required chaperone strand can be inserted into the adhesin or pilin protein, such as FimH, to provide the missing structure and produce the  
15 correct native structure.

Sokurenko *et al.* (1995, *J. Bacteriol.* 177:3680-86) had found that quantitative variations in mannose-sensitive adhesion of *E. coli* are due primarily to structural differences in the FimH adhesin. Further research has shown that the ability of the FimH lectins to interact with monomannosyl residues strongly correlates with their  
20 ability to mediate *E. coli* adhesion to uroepithelial cells so that certain phenotypic variants of type 1 fimbriae may contribute more than others to the virulence of *E. coli* in the urinary tract. (Sokurenko *et al.*, 1997, *J. Biol. Chem.* 272:17880-6). Heretofore, random point mutations in FimH genes that increase binding of the adhesin to mono-mannose residues (structures abundant in the oligosaccharide moieties of urothelial glycoproteins) had been  
25 found to confer increased virulence in the mouse urinary tract (Sokurenko *et al.*, 1998, *Proc. Natl. Acad. Sci. USA* 95:8922-6).

Antibodies directed against purified whole type 1 or P pili protect against cystitis and pyelonephritis, respectively, in both murine and primate models for these diseases. See Abraham *et al.*, 1985, *Infect Immun.* 48:625; Roberts *et al.*, 1994, *Proc. Natl.*  
30 *Acad. Sci. (USA)* 91:11889; and O'Hantey *et al.*, 1985, *J. Clin. Invest.* 75: 347. However, such protection is limited to either homologous *E. coli* strains from which the pili used as immunogens were derived, or to a small subset of serologically cross-reactive heterologous strains. Therefore, vaccines composed predominantly of the major structural proteins of pili (*i.e.*, PapA or FimA) appear to be of limited value because antibodies developed against  
35 these highly variable proteins are specific for the strains used for immunization.



Vaccination techniques have been developed wherein the vaccine composition is delivered to the subject directly at mucosal tissues, such as gut associated lymphoid tissue, nasopharyngeal lymphoid tissue and bronchial-associated lymphoid tissue, thereby providing localized immunity. Mucosal humoral immunity has been generally  
5 thought to come from the secreted form of immunoglobulin, IgA. However, to date, there are no reports of systemic administration of a FimH vaccine composition to a primate which stimulates a humoral immune response sufficient to provide protective immunity at mucosal tissues in humans, with respect to urogenital tract infections. FimH is highly conserved not only among uropathogenic strains of *E. coli*, but also among a wide range of gram-negative  
10 bacteria. For example, all Enterobacteriaceae produce FimH. Thus, vaccines incorporating the FimH antigen should exhibit a broad spectrum of protection.

In addition to vaccination, inhibitory antibodies to FimH may be used in a passive immunization approach to elicit protection from infection. This type of approach has been successful used to combat respiratory syncytial virus (RSV) infection. Newborns  
15 that were given antibodies directed against RSV intravenously and intramuscularly had decreased incidence of RSV infection. This same group of investigators then examined the ability of hyperimmune serum or purified antibody to protect cotton rats and primates against RSV infection (Prince *et al.*, 1985, *Virus Res.* 3:193-206; Prince *et al.*, 1990, *J. Virol.* 64:3091-3092; Hemming *et al.*, 1985, *J. Infect. Dis.* 152:1083-1087; Prince *et al.*,  
20 1983, *Infect. Immun.* 42:81-87; and Prince *et al.*, 1985, *J. Virol.* 55:517-520). Results of these studies suggested that RSV inhibitory antibody given prophylactically inhibited respiratory tract replication of RSV in cotton rats. When given therapeutically, RSV antibody reduced pulmonary viral replication both in cotton rats and in a nonhuman primate model.

While other antigens have been utilized to produce antibodies for diagnosis and for the prophylaxis and/or treatment of bacterial urinary tract infections, there is a need for improved or more efficient vaccines and inhibitory antibodies for use in primates, and more particularly in humans. Such vaccines and inhibitory antibodies should have an improved or enhanced effect in preventing bacterial infections mediated by adhesins and pili  
30 sufficient to prevent or treat UTI in humans.

### 3. BRIEF SUMMARY OF THE INVENTION

Traditional approaches of generating antibody responses to proteins, particularly to inhibit protein function, such as binding to a binding partner, have focused on  
35 targeting antibody responses to either a conserved immunogenic linear epitope, a



conformational epitope that mimics native protein structure, or a surface epitope outside of the binding site. The antibody's blocking effect results from agglutination or steric hindrance. The present invention is based, in part, on the inventors' discovery that mutant forms of the bacterial adhesin FimH, which include one or more mutations in a region of FimH critical to mannose binding, induces antibodies with a greater functional inhibitory activity (in this case binding of FimH to mannose or epithelial cells) than those antibodies induced by wild type FimH. Although not intending to be bound by any mechanism of action, the mutant FimH is predicted to adopt a more open conformation in a region critical for mannose binding such that residues that were poorly exposed in the wild type protein can be exploited as epitopes in the mutant protein. Antibodies directed to these once poorly accessible epitopes are highly inhibitory to the adhesin binding to its cellular receptor.

Accordingly, the present invention relates to methods for inducing antibodies having enhanced functional inhibitory activity, particularly enhanced ability to block binding of a protein to its binding partner, by immunization with a mutant form of the protein (*i.e.*, having one or more amino acid modifications relative to the wild type protein or some other reference protein, which may be another mutant protein), whereby the antibodies elicited by the mutant protein have greater functional inhibitory activity than antibodies elicited by the wild-type or reference protein. In particular embodiments, the protein antigen has one or more mutations relative to the wild type or reference protein, which mutations are in regions of the protein involved in protein function (*e.g.*, ligand or receptor binding) and which regions may be poorly exposed to solvent and/or poorly accessible for antibody production *in vivo* in the wild type protein. The mutations may result in exposing otherwise poorly exposed epitopes that serve as highly potent targets for functional, inhibitory antibodies. In other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations abolish or significantly reduce protein function (for example, but not by way of limitation, binding to a binding partner). In yet other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations result in a protein comprising peptides that bind more tightly to major histocompatibility complex (MHC) molecules resulting in enhanced antigen presentation.

The invention relates to production of high potency inhibitory antibodies against any protein that has a binding partner, for example, against a ligand associated with a receptor-ligand pair, particularly ligands on pathogens involved in binding to host cell receptors. Using pathogen ligands it is possible to develop vaccines that induce antibodies that inhibit binding of the pathogen to host cell receptors, thus preventing infection.



Peptides and proteins that elicit antibodies with greater inhibitory activity and antibodies with greater inhibitory activity are advantageous in that they provide greater protection against infection (or whatever therapeutic or prophylactic effect is desired).

5 A particular embodiment of the invention provides mutant adhesin proteins and peptides that elicit antibodies that have greater activity in inhibiting binding of the adhesin protein, and/or the pathogen associated therewith, to the corresponding cellular receptor of the adhesin protein; as well as antibodies elicited by immunization with such mutant adhesin proteins and peptides. In one embodiment the adhesin molecule is PapG and the binding partner is a Gal $\alpha$ (1-4)Gal.

10 In a preferred embodiment, the invention provides mutant *E. coli* FimH proteins and peptides that elicit antibodies that more effectively inhibit binding of FimH to mannose than antibodies elicited by wild type FimH (or even other reference mutants of FimH). In particular embodiments, the mutations involve one or more amino acid modifications (*e.g.*, insertions, deletions and, preferably, substitutions) in the canyon region  
15 of the FimH molecule, which region is involved in mannose binding. In certain embodiments, the amino acid modifications promote a more open conformation of the FimH protein to expose regions that are poorly exposed in the wild type FimH molecule. In other embodiments, the amino acid modifications significantly reduce or abolish FimH-mannose binding. Preferably, the mutations are made in one or more of amino acid residues  
20 1, 13, 46, 47, 48, 52, 54, 62, 67, 75, 133, 135, 137, 138, 140, 142, 154, 156, and 161 of the FimH amino acid sequence depicted in Figure 1 and in SEQ ID NO:4 (or the corresponding residue in a FimH variant or other adhesin molecule as determined by sequence alignment, *see e.g.*, Figure 3). In a preferred embodiment, the amino acid modification (preferably substitution) is at residue 54, 133, or 135 of the amino acid sequence of FimH (Figure 1  
25 and SEQ ID NO:4). In more preferred embodiments, the amino acid residue at position 54 can be substituted with asparagine or alanine; the residue at amino acid position 133 can be substituted with lysine, arginine, glutamate, or histidine; and/or the amino acid residue at position 135 can be substituted with aspartic acid. Such mutant proteins and peptides are particularly useful as vaccines for the prevention of UTI. Further, the invention  
30 encompasses molecules having two or more mutations wherein one mutation is of amino acid residue 54, 133, or 135 of the FimH amino acid sequence.

Also encompassed by the invention are vaccine compositions comprising the mutant proteins and polypeptides, and antibodies produced by immunizing with such mutant proteins and polypeptides, as well as methods of vaccination, treatment and prophylaxis  
35 using the proteins, polypeptides and antibodies of the invention.



In another embodiment, the antibodies directed against the mutant protein can be administered directly as passive immunization. The present invention is based, in part, on the development of methods for achieving or inducing a prophylactically or therapeutically effective serum titer of an antibody or fragment thereof that  
5 immunospecifically binds to a mutant antigen of a pathogen of interest in a mammal by passive immunization with such an antibody or fragment thereof. The present invention also includes the identification of antibodies with higher inhibitory activity which result in increased efficacy for prophylactic or therapeutic uses such that lower serum titers are prophylactically or therapeutically effective, thereby permitting administration of low  
10 dosages and/or less frequent administration as compared to other antibody therapeutics.

The present invention provides methods of preventing, neutralizing, treating and ameliorating one or more symptoms associated with a pathogen infection in a subject comprising administering to said subject one or more antibodies or fragments thereof which immunospecifically bind to one or more pathogen antigens and display an increased  
15 inhibitory activity. Because a lower serum titer of such antibodies or fragment thereof is therapeutically or prophylactically more effective than the effective serum titer of known antibodies, low to moderate doses of said antibodies or antibody fragments can be used to achieve a serum titer effective for the prevention, neutralization, treatment and the amelioration of symptoms associated with a pathogen infection. The use of low doses of  
20 antibodies or fragments thereof which immunospecifically bind to one or more pathogen antigens reduces the likelihood of adverse effects. Further, the increased inhibitory activity of the antibodies of the invention or fragments thereof enable less frequent administration of said antibodies or antibody fragments than previously thought to be necessary for the prevention, neutralization, treatment or the amelioration of symptoms associated with a  
25 pathogen infection.

The invention further includes co-crystals of a purified FimCH complex bound to a mannose in crystalline form. The invention encompasses the use of the three-dimensional structural representation of this co-crystal to design and/or screen mutant proteins, for example as vaccines, to produce antibodies with these mutant proteins or to  
30 design other molecules as therapeutic or prophylactic candidates for drug development. The designing or screening can be conducted using computers and computational programs or actual synthesis and *in vitro* and/or *in vivo* screening. The invention includes the use of the atomic coordinates representing the three-dimensional structure and a machine-readable medium embedded with information that corresponds to a three-dimensional structural  
35 representation of the FimCH-mannose complex.



In one aspect, the invention provides crystalline forms of polypeptides corresponding to FimCH bound to a mannose sugar. The FimCH complex of the crystalline form can be a wild type FimCH complex or a mutant FimCH complex. The mutant FimCH complex can comprise a mutant FimC or a mutant FimH or both. For example, the mutant FimCH complex can comprise a truncated mutant of FimC or a truncated mutant of FimH, or both. In certain embodiments of the invention, the mutant FimCH complex can be any mutant FimCH complex described herein. In the co-crystals, the mannose sugar can be any mannose sugar including, for example, mannopentaose, methyl-alpha-D-mannopyranoside, alpha-D-mannopyranoside, mannotriose, an oligomannoside, a dimannoside, etc.

The crystals of the invention include native crystals, in which the crystallized FimCH is substantially pure; heavy-atom derivative crystals, in which the crystallized FimCH is in association with one or more heavy-metal atoms; and co-crystals, in which the crystallized FimCH is in association with one or more compounds, including but not limited to, cofactors, ligands, substrates, substrate analogs, inhibitors, allosteric effectors, etc. to form a crystalline co-complex. Preferably, such compounds bind a catalytic or active site. The co-crystals may be native co-crystals, in which the co-complex is substantially pure, or they may be heavy-atom derivative co-crystals, in which the co-complex is in association with one or more heavy-metal atoms.

In one embodiment, wild-type FimCH alpha-D-mannopyranoside co-crystals of the invention are generally characterized by a unit cell of  $a=138.077\pm0.2$  Å,  $b=138.130\pm0.2$  Å,  $c=215.352\pm0.2$  Å,  $\alpha=90$ ,  $\beta=90.005$ ,  $\gamma=90$  and are preferably of diffraction quality. In another embodiment of the invention, FimCH Q133N methyl-alpha-D-mannopyranoside co-crystals of the invention are generally characterized by a unit cell of  $a=138.349\pm0.2$  Å,  $b=138.334\pm0.2$  Å,  $c=213.212\pm0.2$  Å,  $\alpha=90.000$ ,  $\beta=89.983$ ,  $\gamma=90.000$  and are preferably of diffraction quality. In another embodiment of the invention, truncated FimCH mannopentaose co-crystals of the invention are generally characterized by a unit cell of  $a=40.002\pm0.2$  Å,  $b=41.762\pm0.2$  Å,  $c=97.074\pm0.2$  Å,  $\alpha=90$ ,  $\beta=90$ ,  $\gamma=90$  and are preferably of diffraction quality.

In more preferred embodiments, the crystals of the invention are of sufficient quality to permit the determination of the three-dimensional X-ray diffraction structure of the crystalline polypeptide to high resolution, preferably to a resolution of greater than about



3 Å, typically in the range of about 1 Å to about 3 Å, about 1.5 Å to about 3 Å, or about 2 Å to about 3 Å.

The invention also provides methods of making the crystals of the invention. Generally, crystals of the invention are grown by dissolving substantially pure polypeptide  
5 in an aqueous buffer that includes a precipitant at a concentration just below that necessary to precipitate the polypeptide. Water is then removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

Co-crystals of the invention are prepared by soaking a native crystal prepared according to the above method in a liquor comprising the compound of the desired co-  
10 complex. Alternatively, the co-crystals may be prepared by co-crystallizing the polypeptide in the presence of the compound according to the method discussed above.

Heavy-atom derivative crystals of the invention may be prepared by soaking native crystals or co-crystals prepared according to the above method in a liquor comprising a salt of a heavy atom or an organometallic compound. Alternatively, heavy-atom  
15 derivative crystals may be prepared by crystallizing a polypeptide comprising selenomethionine and/or selenocysteine residues according to the methods described previously for preparing native crystals.

In another aspect, the invention provides machine-computer-readable media embedded with the three-dimensional structural information obtained from the crystals of  
20 the invention, or portions or substrates thereof. Such three-dimensional structural information will typically include the atomic structure coordinates of the crystallized polypeptide or co-complex, or the atomic structure coordinates of a portion thereof such as, for example, an active or binding site, but may include other structural information, such as vector representations of the atomic structures coordinates, etc. The types of machine- or  
25 computer-readable media into which the structural information is embedded typically include magnetic tape, floppy discs, hard disc storage media, optical discs, CD-ROM, electrical storage media such as RAM or ROM, and hybrids of any of these storage media. Such media further include paper on which is recorded the structural information that can be read by a scanning device and converted into a three-dimensional structure with an OCR.  
30 The machine readable media of the invention may further comprise additional information that is useful for representing the three-dimensional structure, including, but not limited to, thermal parameters, chain identifiers, and connectivity information.

The invention is illustrated by way of a working example demonstrating the crystallization and characterization of crystals, the collection of diffraction data, and the  
35 determination and analysis of the three-dimensional structure of FimCH.



The atomic structure coordinates and machine readable media of the invention have a variety of uses. For example, the coordinates are useful for solving the three-dimensional X-ray diffraction and/or solution structures of other proteins, including mutant FimCH, co-complexes comprising FimCH, and unrelated proteins, to high  
5 resolution. Structural information may also be used in a variety of molecular modeling and computer-based screening applications to, for example, intelligently design mutants of the crystallized FimCH that have altered biological activity and to computationally design and identify compounds that bind the polypeptide or a portion or fragment of the polypeptide, such as the active site.

### 3.1 DEFINITIONS

The term "analog" as used herein refers to a polypeptide that possesses a similar or identical function as a particular protein (*e.g.*, a FimH polypeptide or FimCH polypeptide complex), or a fragment thereof, but does not necessarily comprise a similar or  
15 identical amino acid sequence or structure of that protein complex or a fragment thereof. A polypeptide that has a similar amino acid sequence refers to a polypeptide that satisfies at least one of the following: (a) a polypeptide having an amino acid sequence that is at least 30%, at least 35%, at least 40%, at least 45%, at least 50%, at least 55%, at least 60%, at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 95%  
20 or at least 99% identical to the amino acid sequence of the protein or protein complex or a fragment thereof as described herein; (b) a polypeptide encoded by a nucleotide sequence that hybridizes under stringent conditions to a nucleotide sequence encoding a protein or protein complex of the invention, or fragment thereof, as described herein of at least 20 amino acid residues, at least 25 amino acid residues, at least 40 amino acid residues, at least  
25 50 amino acid residues, at least 60 amino residues, at least 70 amino acid residues, at least 80 amino acid residues, at least 90 amino acid residues, at least 100 amino acid residues, at least 125 amino acid residues, or at least 150 amino acid residues; and (c) a polypeptide encoded by a nucleotide sequence that is at least 30%, at least 35%, at least 40%, at least 45%, at least 50%, at least 55%, at least 60%, at least 65%, at least 70%, at least 75%, at  
30 least 80%, at least 85%, at least 90%, at least 95% or at least 99% identical to the nucleotide sequence encoding the protein or protein complex of the invention or a fragment thereof as described herein. A polypeptide with similar structure to a protein or protein complex of the invention or a fragment thereof as described herein refers to a polypeptide that has a similar secondary, tertiary or quaternary structure of said protein or protein complex or a fragment  
35 thereof as described herein. The structure of a polypeptide can be determined by methods



known to those skilled in the art, including but not limited to, X-ray crystallography, nuclear magnetic resonance, and crystallographic electron microscopy.

The term "derivative" as used herein refers to a polypeptide that comprises an amino acid sequence of a protein (*e.g.*, FimH) or protein complex (*e.g.*, FimCH) of the invention or a fragment thereof as described herein that has been altered by the introduction of amino acid residue substitutions, deletions or additions. The term "derivative" as used herein also refers to a protein or protein complex of the invention or a fragment thereof that has been modified, *i.e.*, by the covalent attachment of any type of molecule to the polypeptide. For example, but not by way of limitation, a protein or protein complex or a fragment thereof may be modified, *e.g.*, by glycosylation, acetylation, pegylation, phosphorylation, amidation, derivatization by known protecting/blocking groups, proteolytic cleavage, linkage to a cellular ligand or other protein, etc. A derivative of a protein or protein complex or a fragment thereof may be modified by chemical modifications using techniques known to those of skill in the art, including, but not limited to specific chemical cleavage, acetylation, formylation, metabolic synthesis of tunicamycin, etc. Further, a derivative of a protein or protein complex or a fragment thereof may contain one or more non-classical amino acids. A polypeptide derivative possesses a similar or identical function as a protein or protein complex or a fragment thereof described herein.

The term "fragment" as used herein refers to a peptide or polypeptide comprising an amino acid sequence of at least 20 contiguous amino acid residues, at least 25 contiguous amino acid residues, at least 40 contiguous amino acid residues, at least 50 contiguous amino acid residues, at least 60 contiguous amino residues, at least 70 contiguous amino acid residues, at least contiguous 80 amino acid residues, at least contiguous 90 amino acid residues, at least contiguous 100 amino acid residues, at least contiguous 125 amino acid residues, at least 150 contiguous amino acid residues, at least contiguous 175 amino acid residues, at least contiguous 200 amino acid residues, or at least contiguous 250 amino acid residues of the amino acid sequence of a protein of the invention, such as FimH.

An "isolated" or "purified" polypeptide or polypeptide complex of the invention or fragment thereof is substantially free of cellular material or other contaminating proteins from the cell or tissue source from which the protein is derived, or substantially free of chemical precursors or other chemicals when chemically synthesized. The language "substantially free of cellular material" includes preparations of a polypeptide or polypeptide complex in which the polypeptide or polypeptide complex is separated from cellular components of the cells from which it is isolated or recombinantly produced. Thus,



a polypeptide or polypeptide complex that is substantially free of cellular material includes preparations of polypeptide or polypeptide complex having less than about 30%, 20%, 10%, or 5% (by dry weight) of heterologous protein (also referred to herein as a "contaminating protein"). When the polypeptide or polypeptide complex is recombinantly produced, it is also preferably substantially free of culture medium, *i.e.*, culture medium represents less than about 20%, 10%, or 5% of the volume of the protein preparation. When the polypeptide or polypeptide complex is produced by chemical synthesis, it is preferably substantially free of chemical precursors or other chemicals, *i.e.*, it is separated from chemical precursors or other chemicals which are involved in the synthesis of the protein. Accordingly such preparations of the polypeptide or polypeptide complex have less than about 30%, 20%, 10%, 5% (by dry weight) of chemical precursors or compounds other than the polypeptide or polypeptide complex of interest. In a preferred embodiment, polypeptides or polypeptide complexes or fragments thereof of the invention are isolated or purified.

An "isolated" nucleic acid molecule is one which is separated from other nucleic acid molecules which are present in the natural source of the nucleic acid molecule but excludes when the nucleic acid is present as part of a cDNA library. Moreover, an "isolated" nucleic acid molecule, such as a cDNA molecule, can be substantially free of other cellular material, or culture medium when produced by recombinant techniques, or substantially free of chemical precursors or other chemicals when chemically synthesized.

"Plasmids" are designated by a lower case p preceded and/or followed by capital letters and/or numbers. The starting plasmids herein are either commercially available, publicly available on an unrestricted basis, or can be constructed from available plasmids in accord with published procedures. In addition, equivalent plasmids to those described are known in the art and will be apparent to the ordinarily skilled artisan.

The term "attachment domain" refers to the portion of a polypeptide that mediates binding between the polypeptide and a second moiety. The second moiety can comprise cell surface polypeptides and/or polysaccharides. The attachment domain for a FimH polypeptide, which is a type 1 adhesin protein produced by *E. coli*, is depicted in Figure 2E.

The term "canyon region" refers to the region of the FimH polypeptide (or related adhesin) whose surface comprises residues 1, 13, 46, 47, 48, 52, 54, 133, 135, 137, 138, 140, and 142 of FimH (Figure 2) as surface residues of the canyon structure or corresponding residues of a FimH variant or other adhesin as determined by sequence alignment and/or structural comparison.



The term "associated ligand" as used herein refers to a ligand that has an inherent function associated with the recited protein (*e.g.*, binding, such as receptor-ligand binding) and, preferably, does not include an antigen-antibody relationship. As an example, an associated ligand to PapG is a Gal $\alpha$ (1-4)Gal moiety. As another example, an associated  
5 ligand to FimH is a mannose moiety.

The term "periplasmic chaperone" is defined as a protein localized in the periplasm of bacteria that is capable of forming complexes with a variety of chaperone-binding proteins via recognition of a common binding epitope (or epitopes). Chaperones perform several functions. They serve as templates upon which proteins  
10 exported from the bacterial cell into the periplasm fold into their native conformations. Association of the chaperone-binding protein with the chaperone also serves to protect the binding proteins from degradation by proteases localized within the periplasm, increases their solubility in aqueous solution, and leads to their sequentially correct incorporation into an assembling pilus. Chaperone proteins are a class of proteins in gram-negative bacteria  
15 that are involved in the assembly of pili by mediating such assembly, but are not incorporated into the structure. PapD is the periplasmic chaperone protein mediating the assembly of pili for P pilated bacteria and FimC is the periplasmic chaperone protein that mediates assembly of type 1 pili in bacteria.

The term "fusion protein" as used herein refers to a polypeptide that  
20 comprises an amino acid sequence of a polypeptide or fragment thereof and an amino acid sequence of a heterologous polypeptide (*e.g.*, FimH conjugated to FimC).

The term "FimH antigen" refers to a FimH polypeptide or fragment thereof to which an antibody or antibody fragment immunospecifically binds. A FimH antigen also refers to an analog or derivative of a FimH polypeptide or fragment thereof to which an  
25 antibody or antibody fragment immunospecifically binds.

The term "FimCH complex" refers to a complex containing both a FimH and a FimC polypeptide preferably in a 1:1 ratio in the complex.

The terms "pili," "fimbriae," and "fibrillae" are used herein to refer to heteropolymeric protein structures located on the extracellular surface of bacteria, most  
30 commonly gram-negative bacteria. Typically these structures are anchored in the outer membrane. Throughout this specification the terms pilus, pili, fimbriae, and fibrilla will be used interchangeably.

The term "substantially similar structure" as used herein refers to a mutant FimH that, although in a more open conformation, retains the general conformation of the  
35 wild type protein.



The term "antibodies or fragments that immunospecifically bind to a FimH antigen" as used herein refers to antibodies or fragments thereof that specifically bind to a FimH polypeptide or a fragment of a FimH polypeptide and do not non-specifically bind to other polypeptides. Antibodies or fragments that immunospecifically bind to a FimH polypeptide or fragment thereof may have cross-reactivity with other antigens. Preferably, antibodies or fragments that immunospecifically bind to a FimH polypeptide or fragment thereof do not cross-react with other antigens. Antibodies or fragments that immunospecifically bind to a FimH polypeptide can be identified, for example, by immunoassays or other techniques known to those of skill in the art.

The term "Fab fragment" as used herein refers to a fragment of an antibody corresponding to an intact light chain associated with a  $V_H$ - $C_{\gamma 1}$  fragment of the heavy chain. Although these fragments retain the ability to bind antigen, they are no longer bivalent and thus have lost the ability to aggregate antigen. Fab fragments may be generated by any technique known to those of skill in the art. For example, Fab fragments of the invention may be produced by proteolytic cleavage of immunoglobulin molecules, using enzymes such as papain. Techniques to recombinantly produce Fab fragments can also be employed using methods known in the art such as those disclosed in PCT publication WO 92/22324; Mullinax et al., 1992, *BioTechniques* 12:864-869; and Sawai et al., 1995, *AJRI* 34:26-34; and Better et al., 1988, *Science* 240:1041-1043 (said references incorporated herein by reference in their entireties).

The term "functional inhibitory activity" (in some cases "inhibitory activity") means the ability of an antibody to inhibit or reduce the binding of a protein for a binding partner. For example, the functional, inhibitory activity of an anti-FimH antibody is the ability of the antibody to inhibit or reduce the binding of FimH to a mannose moiety (e.g., mono- or tri-mannose).

The term "passive immunization" as used herein refers to the administration of immune serum or purified antibodies or fragments thereof directly to a patient. Immune serum or purified antibodies can be given prophylactically to inhibit infection or therapeutically to reduce or eliminate infection. This is distinguished from immunization of a patient with a protein to direct an *in vivo* immune response to produce antibodies.

To determine the percent identity of two amino acid sequences or of two nucleic acid sequences, the sequences are aligned for optimal comparison purposes (e.g., gaps can be introduced in the sequence of a first amino acid or nucleic acid sequence for optimal alignment with a second amino acid or nucleic acid sequence). The amino acid residues or nucleotides at corresponding amino acid positions or nucleotide positions are



then compared. When a position in the first sequence is occupied by the same amino acid residue or nucleotide as the corresponding position in the second sequence, then the molecules are identical at that position. The percent identity between the two sequences is a function of the number of identical positions shared by the sequences (*i.e.*, % identity =  
5 number of identical overlapping positions/total number of positions x 100%). In one embodiment, the two sequences are the same length.

The determination of percent identity between two sequences can also be accomplished using a mathematical algorithm. A preferred, non-limiting example of a mathematical algorithm utilized for the comparison of two sequences is the algorithm of  
10 Karlin and Altschul, 1990, *Proc. Natl. Acad. Sci. U.S.A.* 87:2264-2268, modified as in Karlin and Altschul, 1993, *Proc. Natl. Acad. Sci. U.S.A.* 90:5873-5877. Such an algorithm is incorporated into the NBLAST and XBLAST programs of Altschul *et al.*, 1990, *J. Mol. Biol.* 215:403. BLAST nucleotide searches can be performed with the NBLAST nucleotide  
15 program parameters set, *e.g.*, for score=100, wordlength=12 to obtain nucleotide sequences homologous to a nucleic acid molecules of the present invention. BLAST protein searches can be performed with the XBLAST program parameters set, *e.g.*, to score=50, wordlength=3 to obtain amino acid sequences homologous to a protein molecule of the present invention. To obtain gapped alignments for comparison purposes, Gapped BLAST can be utilized as described in Altschul *et al.*, 1997, *Nucleic Acids Res.* 25:3389-3402.  
20 Alternatively, PSI-BLAST can be used to perform an iterated search which detects distant relationships between molecules (*Id.*). When utilizing BLAST, Gapped BLAST, and PSI-Blast programs, the default parameters of the respective programs (*e.g.*, of XBLAST and NBLAST) can be used (*e.g.*, <http://www.ncbi.nlm.nih.gov>). Another preferred, non-limiting example of a mathematical algorithm utilized for the comparison of sequences  
25 is the algorithm of Myers and Miller, 1988, *CABIOS* 4:11-17. Such an algorithm is incorporated in the ALIGN program (version 2.0) which is part of the GCG sequence alignment software package. When utilizing the ALIGN program for comparing amino acid sequences, a PAM120 weight residue table, a gap length penalty of 12, and a gap penalty of 4 can be used.

30 The percent identity between two sequences can be determined using techniques similar to those described above, with or without allowing gaps. In calculating percent identity, typically only exact matches are counted.

The term "selenomethionine mutant" as used herein refers to a mutant which includes at least one selenomethionine (SeMet) residue, typically by substitution of a Met  
35 residue of the wild-type sequence with a SeMet residue, or by addition of one or more



SeMet residues at one or both termini. Preferred SeMet mutants are those in which each Met residue is substituted with a SeMet residue.

The term "cysteine mutant" as used herein refers to a mutant in which at least one cysteine residue of the wild-type sequence is replaced with another residue, preferably with a Ser (S) residue. The term can also refer to a mutant in which a non-cysteine residue, preferably a Ser (S) residue, of the wild-type sequence is replaced with a cysteine residue.

The term "selenocysteine mutant" as used herein refers to a mutant which includes at least one selenocysteine (SeCys) residue, typically by substitution of a Cys residue of the wild-type sequence with a SeCys residue, or by addition of one or more SeCys residues at one or both termini. The term can also refer to a cysteine mutant in which at least one Cys residue is substituted with a SeCys residue. Preferred SeCys mutants are those in which each Cys residue is substituted with a SeCys residue.

The term "crystal" as used herein refers to a composition comprising a polypeptide in crystalline form. The term "crystal" includes native crystals, heavy-atom derivative crystals and co-crystals, as defined herein.

The term "native Crystal" as used herein refers to a crystal wherein the polypeptide is substantially pure. As used herein, native crystals do not include crystals of polypeptides comprising amino acids that are modified with heavy atoms, such as crystals of selenomethionine mutants, selenocysteine mutants, etc.

The term "heavy-atom derivative crystal" as used herein refers to a crystal wherein the polypeptide is in association with one or more heavy-metal atoms. As used herein, heavy-atom derivative crystals include native crystals into which a heavy metal atom is soaked, as well as crystals of selenomethionine mutants and selenocysteine mutants.

The term "co-crystal" as used herein refers to a composition comprising a co-complex, as defined above, in crystalline form. Co-crystals include native co-crystals and heavy-atom derivative co-crystals.

The term "diffraction quality crystal" as used herein refers to a crystal that is well-ordered and of a sufficient size, *i.e.*, at least 10 $\mu$ m, preferably at least 50 $\mu$ m, and most preferably at least 100 $\mu$ m in its smallest dimension such that it produces measurable diffraction to at least 3 Å resolution, preferably to at least 2 Å resolution, and most preferably to at least 1.5 Å resolution or lower. Diffraction quality crystals include native crystals, heavy-atom derivative crystals, and co-crystals.

The term "unit cell" as used herein refers to the smallest and simplest volume element (*i.e.*, parallelepiped-shaped block) of a crystal that is completely representative of the unit or pattern of the crystal, such that the entire crystal can be generated by translation of



the unit cell. The dimensions of the unit cell are defined by six numbers: dimensions  $a$ ,  $b$  and  $c$  and angles  $\alpha$ ,  $\beta$  and  $\gamma$  (Blundel *et al.*, 1976, Protein Crystallography, Academic Press.). A crystal is an efficiently packed array of many unit cells.

5 The term "triclinic unit cell" as used herein refers to a unit cell in which  $a \neq b \neq c$  and  $\alpha \neq \beta \neq \gamma$ .

The term "monoclinic unit cell" as used herein refers to a unit cell in which  $a \neq b \neq c$ ;  $\alpha = \gamma = 90^\circ$ ; and  $\beta \neq 90^\circ$ , defined to be  $\geq 90^\circ$ .

10 The term "orthorhombic unit cell" as used herein refers to a unit cell in which  $a \neq b \neq c$ ; and  $\alpha = \beta = \gamma = 90^\circ$ .

The term "tetragonal unit cell" as used herein refers to a unit cell in which  $a = b \neq c$ ; and  $\alpha = \beta = \gamma = 90^\circ$ .

The term "trigonal/rhombohedral unit cell" as used herein refers to a unit cell in which  $a = b = c$ ; and  $\alpha = \beta = \gamma \neq 90^\circ$ .

15 The term "trigonal/hexagonal unit cell" as used herein refers to a unit cell in which  $a = b = c$ ;  $\alpha = \beta = 90^\circ$ ; and  $\gamma = 120^\circ$ .

The term "cubic unit cell" as used herein refers to a unit cell in which  $a = b = c$ ; and  $\alpha = \beta = \gamma = 90^\circ$ .

The term "crystal lattice" as used herein refers to the array of points defined by the vertices of packed unit cells.

20 The term "space group" as used herein refers to the set of symmetry operations of a unit cell. In a space group designation (*e.g.*, C2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance.

25 The term "asymmetric unit" as used herein refers to the largest aggregate of molecules in the unit cell that possesses no symmetry elements that are part of the space group symmetry, but that can be juxtaposed on other identical entities by symmetry operations.

30 The term "crystallographically-related dimer" as used herein refers to a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer coincide with the symmetry axes or planes of the crystal lattice.

The term "non-crystallographically-related dimer" as used herein refers to a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer do not coincide with the symmetry axes or planes of the crystal lattice.

35 The term "isomorphous replacement" as used herein refers to the method of using heavy-atom derivative crystals to obtain the phase information necessary to elucidate



the three-dimensional structure of a crystallized polypeptide (Blundel *et al.*, 1976, Protein Crystallography, Academic Press.).

The terms "multi-wavelength anomalous dispersion" or "MAD" as used herein refers to a crystallographic technique in which X-ray diffraction data are collected at several different wavelengths from a single heavy-atom derivative crystal, wherein the heavy atom has absorption edges near the energy of incoming X-ray radiation. The resonance between X-rays and electron orbitals leads to differences in X-ray scattering from absorption of the X-rays (known as anomalous scattering) and permits the locations of the heavy atoms to be identified, which in turn provides phase information for a crystal of a polypeptide. A detailed discussion of MAD analysis can be found in Hendrickson, 1985, *Trans. Am. Crystallogr. Assoc.*, 21:11; Hendrickson *et al.*, 1990, *EMBO J.* 9:1665; and Hendrickson, 1991, *Science* 4:91.

The terms "single wavelength anomalous dispersion" or "SAD" as used herein refers to a crystallographic technique in which X-ray diffraction data are collected at a single wavelength from a single native or heavy-atom derivative crystal, and phase information is extracted using anomalous scattering information from atoms such as sulfur or chlorine in the native crystal or from the heavy atoms in the heavy-atom derivative crystal. The wavelength of X-rays used to collect data for this phasing technique need not be close to the absorption edge of the anomalous scatterer. A detailed discussion of SAD analysis can be found in Brodersen *et al.*, 2000, *Acta Cryst.*, D56:431-441.

The terms "single isomorphous replacement with anomalous scattering" or "SIRAS" as used herein refers to a crystallographic technique that combines isomorphous replacement and anomalous scattering techniques to provide phase information for a crystal of a polypeptide. X-ray diffraction data are collected at a single wavelength, usually from a single heavy-atom derivative crystal. Phase information obtained only from the location of the heavy atoms in a single heavy-atom derivative crystal leads to an ambiguity in the phase angle, which is resolved using anomalous scattering from the heavy atoms. Phase information is therefore extracted from both the location of the heavy atoms and from anomalous scattering of the heavy atoms. A detailed discussion of SIRAS analysis can be found in North, 1965, *Acta Cryst.* 18:212-216; Matthews, 1966, *Acta Cryst.* 20:82-86.

The term "molecular replacement" as used herein refers to the method of calculating initial phases for a new crystal of a polypeptide whose structure coordinates are unknown by orienting and positioning a polypeptide whose structure coordinates are known within the unit cell of the new crystal so as to best account for the observed diffraction pattern of the new crystal. Phases are then calculated from the oriented and positioned



polypeptide and combined with observed amplitudes to provide an approximate Fourier synthesis of the structure of the polypeptides comprising the new crystal. (Lattman, 1985, *Methods in Enzymology* 115:55-77; Rossmann, 1972, "The Molecular Replacement Method," Int. Sci. Rev. Ser. No. 13, Gordon & Breach, New York.).

5           The term "having substantially the same three-dimensional structure" as used herein refers to a polypeptide that is characterized by a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2 Å, or less than or equal to about 1 Å, when superimposed onto the atomic structure coordinates of Table 14 when at least about 50% to 100% of the C $\alpha$  atoms of the coordinates are included  
10 in the superposition.

The term "C $\alpha$ " as used herein refers to the alpha carbon of an amino acid residue.

#### 4. BRIEF DESCRIPTION OF THE DRAWINGS

15           Figures 1 A-D: Wild type FimC and FimH nucleic and amino acid sequence. (A) nucleic acid sequence of FimC (SEQ ID NO:1); (B) amino acid sequence of FimC (SEQ ID NO:2); (C) nucleic acid sequence of FimH (SEQ ID NO:3); (D) amino acid sequence of FimH (SEQ ID NO:4) (from Choudhury et al. 1999, *Science* 285:1061 incorporated herein by reference).

20           Figures 2 A-E: Crystal structure of FimCH chaperone-adhesin complex bound to  $\alpha$ -D-mannose. (A) Overall structure of FimCH with the two domains of the chaperone FimC (black) and the pilin domain of FimH (gray). As demonstrated previously, the receptor-binding domain of FimH is an elongated eleven-stranded  $\beta$ -barrel comprised of residues  
25 Phe1 to Thr158, and is connected via a flexible linker to the pilin domain of FimH. (B) The bound mannose receptor is shown at a 90° rotation of the receptor binding domain shown in (A). The mannose, the mannose-interacting residues, and the residues of the hydrophobic ridge around the pocket are shown in ball-and stick model. (C) Stereo  
30 presentation of omit electron density at 4  $\sigma$  ( $F_o - F_c$ ) for the  $\alpha$ -D-mannoside bound in pocket of FimH. The interacting amino acids are shown in ball-and-stick with hydrogen bonds shown by dotted lines. (D) The receptor binding domain of FimH displaying the electrostatic potential surface, with positively and negatively charged residues shaded and hydrophobic residues labeled. (E) The tip of the FimH receptor binding domain is shown.

35           Figure 3: Alignment of deduced amino acid sequences of the FimH lectin-binding



domain from representative clinical isolates. The regions involved in mannose binding are shown highlighted in gray. The other positions shown were found to be heterogenous among throughout all the FimH sequences examined. The sequences that are not shown were found to be conserved also among all isolates. UTI strain J96 was used as the  
 5 consensus sequence. Amino acid residues that are identical to that of J96 were indicated by “.” while the residues different from the consensus were indicated.

Figure 4: FimH mutants were complexed with FimC, another type 1 pilus protein. Wild type FimC was found to associate with wild type FimH, the vaccine composition of  
 10 wild type FimH, FimH N46A, FimH N46D, FimH Q133K, and FimH D140E equally well as assayed by ELISA using an anti-FimC antibody. closed circles=FimH N46A; open circles=FimH D140E; closed triangles=FimH Q133K; open triangles=FimH N46D; closed squares=vaccine composition of wild type FimH; open squares=wild type FimH.

Figures 5 A-B: Binding of purified FimCH complexes to mono-mannose coated beads and their elution by methyl- $\alpha$ -D-mannopyranosides. (A) A Coomassie-stained SDS-PAGE gel shows that most FimH mutants still retained the ability to bind mono-mannose coated beads (“bound”). (A) A Coomassie-stained SDS-PAGE gel shows that bound mutant FimH proteins were eluted-off with methyl- $\alpha$ -D-mannopyranosides (“eluted”). (B)  
 15 The ratio of bound to eluted FimH protein. Asterisk indicates no FimH was bound to the bead initially.

Figures 6 A-B: Binding of purified FimCH complexes to mannose as assayed by ELISA. Comparison of different mutant FimCH proteins in their ability to bind (A) mono-mannose and (B) tri-mannose. In upper panels, closed square with unbroken line=WT control, closed diamond with dotted line=N46D, closed circle=D54A, closed  
 25 triangle=D54N, closed square with dashed line=S62A, opened circle=Q133K, closed upside down triangle=Q133N, closed diamond with dashed line=Q133A, half filled diamond=N135D, bottom filled square=N135A, top filled square=D140N, star=D140A, and open triangle=D140E. In lower panels, closed circle and open square=WT control, open circle=I13A, closed upside down triangle=Y48A, open upside down triangle=I52A, closed square=Q133E, closed diamond=Q133H, open diamond=Q133R, filled triangle=N135D, open triangle=Y137A.



Figures 7 A-I: Mutant FimH expressing *E. coli* binding to mannose. Comparison of different mutant FimCH proteins in their ability to bind (A) monomannose and (B) trimannose. Comparison of monomannose and trimannose binding of PmmB66 expressing wild type FimCH with (C) untransfected PmmB66; (D) PmmB66 expressing FimCH N46A; (E) PmmB66 expressing FimCH N46D; (F) PmmB66 expressing FimCH D140E; (G) PmmB66 expressing FimCH Q133K; and (H) PmmB66 expressing FimCH S62A. (I) Mutant FimH expressing *E. coli* binding to control plates coated with the polyclonal anti-*E. coli* antibody. In panels A, B, and I, closed circle=PmmB66FimH, open circle=WT FimH, filled triangle=N46A, open triangle=N46D, closed square=D140E, open square=Q133K, diamond=S62A. In panels C-H, closed triangle=WT FimH binding to mono-mannose, open triangle=WT FimH binding to tri-mannose, closed circle=FimH binding to mono-mannose, open circle=FimH binding to tri-mannose.

Figures 8 A-B: Binding and invasion of 5637 cells. (A) AAEC185/pUT2002 bacteria complemented with different FimH variants did not exhibit any significant binding to 5637 cells with the exception of FimCH S62A and FimCH N46D mutants. Results were obtained from at least two different infection experiments with duplicate wells in each experiment. X-axis represents the percent cell association of total input bacteria, which includes both the surface bound and invaded bacteria. (B) Bound bacteria expressing mutant FimH proteins showed a similar degree of invasion into 5637 cells. Results shown are from one representative experiment.

Figures 9 A-K: Binding of type 1 pilated-bacteria to human bladder sections. AAEC185/pUT2002 bacteria complemented with (A) WT; (C) S62A; (E) N46A; (F) N46D; (H) D54A; (I) Q133A; and (J) Q133K, FimH expression and (K) vector control plasmids were used in the binding assay. Binding of (B) WT; (D) S62A; and (G) N46D can be inhibited by methyl- $\alpha$ -D-mannopyranosides.

Figures 10 A-C: Results from an ELISA of levels of anti-FimH specific IgG polyclonal antibodies in serum of vaccinated mice. Titers are shown as endpoint dilutions which are measured by an ELISA where FimH T3 (a histidine-tagged fusion protein composed of the first 165 amino acids of FimH) is the capture antigen and the detection antibody is specific to IgG. A booster immunization was given 3 weeks after the initial immunization. Doses of protein at each injection were either 4.0, 1.6, 0.64, and 0.26  $\mu$ g (as indicated). Wild type FimCH was used as an immunogen for vaccination and resulting



antibody titers were compared to those seen for mutant protein: (A) FimCH N46D; (B) FimCH D140E; and (C) FimCH Q133K. WT FimCH is depicted by open symbols while indicated mutant FimCH is depicted by closed symbols. square=4ug, circle=1.6ug, triangle=0.64 ug, diamond=.026 ug. star=MF 59 adjuvant alone.

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Figures 11 A-C: Hemagglutination assay inhibition by polyclonal antibodies. *E. coli* was preincubated with increasing dilutions of a polyclonal antibody raised against the indicated FimCH complex. The FimCH complex on the bacteria was tested for its ability to bind the mannose present on the erythrocytes in the presence of the polyclonal antibody. Decreased mean channel fluorescence in the presence of the antibody indicated that the polyclonal antibody inhibited FimCH binding in this assay. Preincubation with polyclonal antibodies raised against (A) FimCH Q133 E, FimCH Q133H, and WT FimCH and (C) FimCH N135D, FimCH Q133R, and WT FimCH inhibited bacteria binding to the erythrocytes very strongly. (B and D) Control antiserum from animals that were either not immunized or immunized with MF59 adjuvant alone showed no inhibition.

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Figures 12 A-E: Polyclonal antibody inhibition of *E. coli* NU14 binding to J82 human bladder cells as measured by multiple channel fluorescence (MCF) in log2 scale. Polyclonal antibodies raised against the indicated mutant or wild type FimCH protein were preincubated with bacteria cells before addition to bladder cells for binding: (A) anti-FimCH N46D (8 week sera used after a boost at week 4); (B) anti-FimCH D140E (8 week sera used after a boost at week 4); and (C) anti-FimCH Q133K (8 week sera used after a boost at week 4). For wild type FimCH and FimCH Q133K, an additional boost at week 18 was given. Inhibitory assays were done with antisera from week 16 (darker bar) and week 20 (lighter bar): (D) anti FimCH; and (E) anti-FimCH Q133K.

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Figure 13: Passive immunization with polyclonal antibodies generated with mutant FimCH protein. Mice were administered 1 mg of polyclonal antibody 4 hours prior to a large bolus challenge with *E. coli* Nu14. After 48 hours, mice were sacrificed to harvest the bladders. The number of CFUs were determined. A decrease in the number of CFUs indicates that the passive immunization had a protective ability.

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Figure 14: Hemagglutination assay inhibition by monoclonal antibody (MAB). *E. coli* was preincubated with increasing dilutions of the indicated MAB clone. The FimCH complex on the bacteria was tested for its ability to bind the mannose present on the

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erythrocytes in the presence of the MAB. Decreased mean channel fluorescence indicated that the MAB clone was inhibitory in this assay. Preincubation with clone 1A7 inhibited bacteria binding to the erythrocytes very strongly. Clones 1C10 and 3E11 also inhibited bacteria binding when the MABs were supplied in larger quantities. Clones 1F2, 2B2, and 1C8 did not show an inhibitory activity.

Figure 15: Hemagglutination assay inhibition by MAB clone 1A7. *E. coli* was preincubated with increasing dilutions of MAB clone 1A7. The FimCH complex on the bacteria was tested for its ability to bind the mannose present on the erythrocytes in the presence of the MAB. Decreased mean channel fluorescence indicated that the MAB clone was inhibitory in this assay. (A) Preincubation with clone 1A7 inhibited bacteria binding to the erythrocytes very strongly. (B) Controls showed that this inhibitory activity was due to preincubation with MAB clone 1A7.

Figure 16: Tri-mannose binding inhibition by MAB. An ELISA assay was used to measure the ability of the FimCH complex on bacteria to bind tri-mannose in the presence of the MAB. A decrease in OD<sub>450</sub> indicated that bacteria were inhibited from binding to the tri-mannose. Both MAB clone 1A7 and 1C10 inhibited binding while MAB clone 1C8 did not. closed circle=1A7, open circle=1C8, upside down triangle=1C10, triangle=anti B19 negative control.

Figure 17: Hemagglutination assay inhibition by Fab fragments. *E. coli* was preincubated with increasing dilutions of the indicated Fab fragment. The FimCH complex was tested for its ability to bind the mannose present on the erythrocytes in the presence of the Fab fragment. Decreased mean channel fluorescence indicates that the Fab fragment was inhibitory in this assay.

Figure 18: Passive immunization with MABs generated with mutant FimCH protein. Mice were administered 1 mg of MAB 4 hours prior to a large bolus challenge with *E. coli* Nu14. After 48 hours, mice were sacrificed to harvest the bladders. The number of CFUs were determined. A decrease in the number of CFUs indicates that the passive immunization had a protective ability.

Figures 19 A-B: Ball-and-stick presentation of changes in the structure of the mannose binding pocket between (A) wild type FimCH and (B) Q133N FimCH: Hydrogen



bonds are shown as dotted lines and aromatic contacts are shown as dashed lines. Water molecules are labeled as W1 and/or W2.

## 5. DETAILED DESCRIPTION OF THE INVENTION

5           The present invention is based, in part, on the inventors' discovery that certain mutant forms of the bacterial adhesin FimH, which have one or more mutations in a canyon region of FimH critical to mannose binding, induced antibodies with a greater functional inhibitory activity (in this case inhibiting binding of FimH to mannose or epithelial cells) than those antibodies induced by wild type FimH. Although not intending to  
10 be bound by any mechanism of action, the mutant FimH is predicted to adopt a more open conformation in a region critical for mannose binding such that residues that were poorly exposed in the wild type protein can be exploited as epitopes in the mutant protein. Antibodies directed to these once inaccessible epitopes are highly inhibitory to the adhesin.

          Accordingly, the present invention relates to methods for inducing antibodies  
15 having enhanced functional inhibitory activity, particularly enhanced ability to block binding of a protein to its binding partner, by immunization with a mutant form of the protein (*i.e.*, having one or more amino acid modifications relative to the wild type protein or some other related reference protein, which may be another mutant protein), whereby the antibodies elicited by the mutant protein have greater functional inhibitory activity than antibodies  
20 elicited by the wild-type or reference protein. In particular embodiments, the protein antigen has one or more mutations relative to the wild type or reference protein, which mutations are in regions of the protein involved in protein function (*e.g.*, ligand or receptor binding) and which regions may be poorly exposed to solvent and/or poorly accessible for antibody production *in vivo* in the wild type protein. The mutations may result in exposing otherwise  
25 buried epitopes that serve as highly potent targets for functional, inhibitory antibodies. In other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations abolish or significantly reduce protein function (for example, but not by way of limitation, binding to a binding partner). In yet other embodiments, the protein antigen has one or more mutations relative to the wild type protein or reference  
30 protein, which mutations result in a protein comprising peptides that bind more tightly to MHC molecules resulting in enhanced antigen presentation.

          The invention relates to production of high potency inhibitory antibodies against any protein that has a binding partner, for example, against a ligand associated with a receptor-ligand pair, particularly ligands on pathogens involved in binding to host cell  
35 receptors. Using pathogen ligands is it possible to develop vaccines that induce antibodies



that inhibit binding of the pathogen to host cell receptors, thus preventing infection. Additionally, the antibodies directed against the pathogen protein can be administered directly as passive immunization. Peptides and proteins that elicit antibodies with greater inhibitory activity and antibodies with greater inhibitory activity are advantageous in that they provide greater protection against infection (or whatever therapeutic or prophylactic effect is desired).

Each of the above-described peptides and proteins can be designed or generated using information from the complex of FimCH-mannose in crystalline form, such information includes but is not limited to the three-dimensional structure. Thereafter, antibodies to the novel mutant peptides or proteins can be generated.

### 5.1 MUTANT PROTEINS AS ANTIGENS FOR HIGH POTENCY INHIBITORY ANTIBODIES

The present invention relates to methods for inducing antibodies having enhanced functional inhibitory activity, particularly enhanced ability to block binding of a protein to its binding partner, by immunization with a mutant form of the protein (*i.e.*, having one or more amino acid modifications relative to the wild type protein or some other related reference protein, which may be another mutant protein), whereby the antibodies elicited by the mutant protein have greater functional inhibitory activity than antibodies elicited by the wild-type or reference protein.

In particular embodiments, the protein antigen has one or more mutations relative to the wild type or reference protein, which mutations are in regions of the protein involved in protein function (*e.g.*, ligand or receptor binding) and which regions are poorly exposed to solvent and/or poorly accessible for antibody production *in vivo* in the wild type protein. The mutations may result in exposing otherwise poorly exposed epitopes that serve as highly potent targets for functional, inhibitory antibodies. Such residues can be identified by any means known in the art, preferably, by computer modeling, to identify residues critical for a particular protein conformation, which residues, when modified (preferably, substituted with another amino acid residue), result in a more open protein conformation. In preferred embodiments, the more open protein conformation exposes one or more regions of the protein that are poorly exposed in the wild type or reference protein, more preferably, these one or more regions are involved (in some aspects, critical for) protein binding to a binding pair. Preferably, the amino acid residue that is substituted differs in hydrophobicity, polarity, size, or charge from the amino acid present at that position in the wild type or reference protein. Additionally, libraries of random mutants can be generated at one or more



residues identified by modeling or other methods to be critical for protein conformation, particularly in regions important in protein binding to a binding partner (*e.g.*, ligand binding to an associated receptor), and/or the mutation of which is predicted to expose otherwise poorly exposed regions, preferably those involved in protein binding. Such libraries of randomly mutated proteins can be screened using methods well known in the art for mutant proteins that elicit antibodies that have higher functional inhibitory activity than the antibodies elicited by a wild type or reference protein.

In other embodiments, the protein antigen has one or more mutations (*i.e.*, amino acid modifications) relative to the wild type protein, which mutations abolish or significantly reduce protein function (for example, but not by way of limitation, binding to a binding partner). The residues to be mutated can be identified by any method known in the art for identifying residues critical for ligand binding, for example, but not by way of limitation, protein modeling and mutational analysis. Preferably, the amino acid residue that is substituted differs in hydrophobicity, polarity, size, or charge from the amino acid present at that position in the wild type or reference protein. Additionally, libraries of random mutants can be generated at one or more residues identified by modeling or other methods to be critical for ligand binding. Such libraries of randomly mutated protein can be screened for mutant proteins that have reduced or no binding activity and/or the ability to elicit antibodies that have higher functional inhibitory activity than the antibodies elicited by a wild type or reference protein.

In yet other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations result in a protein-comprising peptides that bind more tightly to MHC molecules resulting in enhanced antigen presentation.

The mutant proteins of the invention may have any number of mutations relative to the corresponding wild type protein or reference protein as long as they elicit antibodies that have greater functional inhibitory activity than antibodies elicited by the wild type or reference protein. In certain embodiments, the protein contains 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 20 or more than 25 mutations. In certain embodiments, the protein also contains mutations relative to the wild type or reference protein that do not affect (or even decrease) the ability of the protein to elicit antibodies with a greater functional inhibitory activity than those elicited by the wild type or reference protein, as long as the mutant protein is able to elicit such high potency inhibitory antibodies. The invention also includes fragments of the mutant proteins that elicit antibodies with greater inhibitory activity than the wild type or reference protein and/or than the corresponding fragment of the wild type or reference protein.



The invention relates to producing mutants of any protein that is a member of a binding pair, including proteins that bind non-protein molecules, such as carbohydrates including lectins, lipids, steroids, non-peptide hormones, or other small molecules. In particular, such proteins are members of a ligand-receptor pair. Either the ligand or the receptor may be the antigen that is mutated. Such mutated ligand or receptor can then be used to raise antibodies with enhanced activity to block ligand-receptor binding. In a preferred embodiment, the binding pair is not an antigen-antibody binding pair.

In preferred embodiments, the invention relates to methods for inducing antibodies having enhanced functional inhibitory activity, particularly enhanced ability to block binding of a pathogenic protein to its host cell receptor, by immunization with a mutant form of the pathogenic protein (*i.e.*, having one or more amino acid modifications relative to the wild type or reference protein), whereby the antibodies elicited by the mutant pathogenic protein have greater functional inhibitory activity than antibodies elicited by the wild-type protein. In particular embodiments, the pathogenic protein antigen has one or more mutations relative to the wild type or reference pathogenic protein, which mutations result in exposing regions of the protein which are poorly exposed to solvent and/or not accessible for antibody production *in vivo* in the wild type protein. By way of example but not limitation, the mutations may result in exposing otherwise poorly exposed epitopes that serve as highly potent targets for antibodies that inhibit binding of pathogenic proteins to host cell receptors.

A particular embodiment of the invention provides methods for inducing antibodies having enhanced ability to block binding of a parasitic ligand to its host cell receptor, by immunization with a mutant form of the parasitic ligand (*i.e.*, having one or more amino acid modifications relative to the wild type or reference ligand), whereby the antibodies elicited by the mutant ligand have greater functional inhibitory activity than antibodies elicited by the wild-type or reference ligand. In particular embodiments, the parasitic ligand has one or more mutations relative to the wild type or reference parasitic ligand, which mutations result in exposing regions which are poorly exposed to solvent and/or poorly accessible for antibody production *in vivo* in the wild type ligand.

Highly preferred embodiments of the invention provide methods for inducing antibodies having enhanced ability to block binding of a microbial adhesin protein to its host cell receptor, by immunization with a mutant form of the adhesin protein, which mutants induce of antibodies with greater inhibitory activity than antibodies elicited by the wild-type adhesin protein. In particular embodiments, the adhesin protein has one or more mutations relative to the wild type or a reference adhesin, which mutations result in exposing regions



of the protein which are poorly exposed in the wild type protein. In other embodiments, the mutations significantly reduce or abolish binding of the adhesin to its host cell surface receptor.

Accordingly, the present invention also relates to antibodies that target  
5 protein binding interactions including but not limited to examples such as antibodies that target  $\alpha V\beta 3$  integrin, FimH, FimCH, and RSV. Embodiments provide antibodies that immunospecifically bind a member of a binding pair. The binding pair can be any two molecules that specifically interact with each other. In specific embodiments, the one  
10 member of the binding pair is an antigen of an infectious disease agent (*i.e.*, a molecule on the surface of an infectious disease agent) or a cellular receptor for an infectious disease agent. Such antigens of infectious disease agents include FimH of *E. coli*, and antigens of HSV-2, gonococcus, *Treponema pallidum*, *Chlamydia trachomatis* or human papillomavirus. The first member of the binding pair can also be a cancer antigen (*i.e.*, a molecule expressed  
15 on the surface of a cancer cell). Such cancer antigens include human milk fat globule antigen (HMFG), an epitope of polymorphic epithelial mucin antigen (PEM), or a human colon carcinoma-associated protein antigen.

The invention further provides methods of treatment or prevention using the antibodies of the invention as discussed herein. For example, peptides to elicit antibodies or  
20 antibodies directed to an infectious agent or a cellular receptor for an infectious disease agent or a cancer antigen can be used in the treatment or prevention of an infectious disease or a cancer associated with the expression of the particular antigen of the infectious disease agent or the cellular receptor for the infectious disease agent.

In a preferred embodiment of the invention, antibodies to mutant adhesin  
25 proteins are generated to inhibit binding of adhesins to cellular receptors. In particular, FimH proteins are responsible for the adhesin binding of type 1 pili to bladder epithelial cells. Accordingly, the invention provides mutant forms of FimH (relative to the FimH amino acid sequence of Figure 1 (SEQ ID NO:3) or corresponding FimH variant of Figure 3) or other bacterial adhesin (*e.g.*, PapG) that elicit antibodies that have greater inhibitory  
30 activity (that prevents binding of the bacteria or the isolated adhesin to the cellular receptor (mannose moieties in the case of FimH) or host cell (bladder epithelial cells in the case of FimH) than antibodies elicited by wild type or a reference FimH or other bacterial adhesin. Without being limited by theory, the invention provides mutant forms of FimH in which the canyon region of FimH, which is involved in mannose binding, adopts a more open  
35 conformation, exposing regions that are poorly exposed in wild type FimH. FimH residues involved in maintaining the canyon structure and/or that, when mutated, would result in



exposing poorly exposed regions in the wild type FimH may be identified by any method known in the art. For example, such residues may be identified by protein modeling. The crystal structure for the FimCH complex is depicted in Choudhury et al., 1999, *Science* 285:1061-1066, which is hereby incorporated by reference in its entirety. More importantly, the crystal structure of the mannose binding pocket of FimH has been determined by co-crystallizing a highly purified FimCH chaperone-adhesin complex together with D-mannose (see Figure 2).

In other embodiments, mutant FimH proteins, or other bacterial adhesins, are provided where one or more amino acid modifications are introduced into the FimH protein that significantly reduce or abolish binding of FimH to mannose or the other bacterial adhesin to its cell surface receptor. In either embodiment, the residues to be modified may be identified through protein modeling and/or analysis of site specific or naturally occurring or any other mutants to identify residues that, when mutated, alter protein structure or binding of the protein to its cellular receptor. In certain embodiments, libraries of mutant adhesins having random mutations at one or more residues are screened for mutant adhesins in which poorly exposed mutant regions are exposed, mutant adhesins that lack or have significantly reduced binding to the cellular receptor, and/or mutant adhesins that can elicit antibodies that have greater functional inhibitory activity than antibodies elicited by the wild type or reference adhesin.

In preferred embodiments, the mutant protein of the invention is a mutant FimH protein having one or more amino acid modifications (preferably substitutions) at one or more of residues 1, 2, 3, 4, 10, 11, 12, 13, 14, 15, 16, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 77, 78, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145 or 146 of the FimH amino acid sequence in Figure 1 (SEQ ID NO:3) (the residue numbers discussed herein all refer to the residues as numbered on the FimH sequence of Figure 1, unless specifically noted and intend to include corresponding residues in a variant of FimH, as determined by sequence alignment with the amino acid sequence in Figure 1). In a more preferred embodiment, the amino acid modifications (preferably substitutions) are made at one or more of residues 1, 2, 13, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 77, 78, 101, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143 or 144 of the amino acid sequence of FimH in Figure 1 (SEQ ID NO:3). In yet another embodiment, the amino acid modifications (preferably substitutions) are made at one or more of residues 1, 45, 46, 47, 52, 53, 54, 55, 56, 93, 94, 95, 133, 134 or 135 of the amino acid sequence of FimH (Figure 1). In another embodiment, the amino acid modifications (preferably



substitutions) are made at one or more of residues 1, 3, 44, 54, 133, 135, 140, 142 and 144 of the amino acid sequence of FimH ( Figure 1). In a preferred embodiment, the amino acid modification (preferably substitution) is at residue 54, 133, or 135 of the amino acid sequence of FimH ( Figure 1), more preferably where the residue at position 54, 133, or 135 is substituted with a charged residue (in other embodiments substituted with an amino acid having greater steric effects than the wild type residue). In more preferred embodiments, the amino acid residue at position 54 can be substituted with asparagine or alanine; the residue at amino acid position 133 can be substituted with lysine, arginine, glutamate, or histidine; and/or the amino acid residue at position 135 can be substituted with aspartic acid. In other embodiments, the FimH amino acid modifications are in canyon region of FimH, preferably where the canyon region has a surface of residues 1, 13, 46, 47, 48, 52, 54, 133, 135, 137, 138, 140 and 142.

In one embodiment, the site of one or more of the amino acid modifications occurs at a residue that interacts with mannose *e.g.*, as determined by molecular modeling using the crystal structure provided in Figure 2, or the crystal structure in Choudhury et al. 1999, (*Science* 285:1061-1066, incorporated by reference herein in its entirety) or both. Further, the mutations can similarly be made by modeling based upon related crystal structures such as that disclosed herein as Figure 2 and in application no. 09/637,216 filed August 11, 2000, entitled "Anti-Bacterial Compounds Directed vs Pilus Biogenesis, Adhesion and Activity; Co-crystals of Pilus Subunits and Methods of Use" by Hultgren et al., which is herein incorporated by reference.

For example, the modification is made at one or more residues 1, 46, 47, 54, 133, 135, 140, and 142 of FimH (SEQ ID NO:3), which interact with mannose as shown in Table 1.

Table 1: FimH Amino Acid Residues Which Interact with Mannose

residue position	amino acid residue
1	phenylalanine (F)
46	asparagine (N)
47	aspartic acid (D)
54	aspartic acid (D)
133	glutamine (Q)
135	asparagine (N)



140	aspartic acid (D)
142	phenylalanine (F)

In another embodiment, the site of one or more of the amino acid modifications occurs within the hydrophobic ring surrounding the mannose-binding pocket of FimH. For example, residues 13, 48, 52, and 142 of FimH (SEQ ID NO:3), as shown in Table 2.

Table 2: FimH Amino Acid Residues of the Hydrophobic Ring

residue position	amino acid residue
13	isoleucine (I)
48	tyrosine (Y)
52	isoleucine (I)
142	phenylalanine (F)

In one embodiment, the site of one or more of the amino acid modifications occurs within about 15 angstroms from the  $\alpha$  carbon residue 54 of FimH, *e.g.*, as determined by molecular modeling using the crystal structure provided in Figure 2 and in Choudhury et al. 1999, (*Science* 285:1061-1066, incorporated by reference herein in its entirety). For example, the modification is made at one or more residues 1, 2, 3, 4, 10, 11, 12, 13, 14, 15, 16, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 77, 78, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145 and 146 of FimH (SEQ ID NO:3). (see Table 3)

Table 3: Residues 15 angstroms from the  $\alpha$  carbon of residue 54 in FimH

residue position	wild type amino acid
1	phenylalanine (F)
2	alanine (A)
3	cysteine (C)
4	lysine (K)
10	alanine (A)



	11	isoleucine (I)
	12	proline (P)
	13	isoleucine (I)
5	14	glycine (G)
	15	glycine (G)
	16	glycine (G)
	42	isoleucine (I)
10	43	phenylalanine (F)
	44	cysteine (C)
	45	histidine (H)
	46	asparagine (N)
15	47	aspartic acid (D)
	48	tyrosine (Y)
	49	proline (P)
	50	glutamic acid (E)
20	51	asparagine (N)
	52	isoleucine (I)
	53	threonine (T)
	54	aspartic acid (D)
25	55	tyrosine (Y)
	56	valine (V)
	57	threonine (T)
	58	leucine (L)
	59	glutamine (Q)
30	78	serine (S)
	89	glutamic acid (E)
	90	threonine (T)
	91	proline (P)
35	92	arginine (R)



	93	valine (V)
	94	valine (V)
	95	tyrosine (Y)
5	96	asparagine (N)
	97	serine (S)
	98	arginine (R)
	99	threonine (T)
10	101	lysine (K)
	102	proline (P)
	103	tryptophan (W)
	104	proline (P)
15	105	valine (V)
	130	isoleucine (I)
	131	leucine (L)
	132	arginine (R)
20	133	glutamine (Q)
	134	threonine (T)
	135	asparagine (N)
	136	asparagine (N)
25	137	tyrosine (Y)
	138	asparagine (N)
	139	serine (S)
	140	aspartic acid (D)
30	141	aspartic acid (D)
	142	phenylalanine (F)
	143	glutamine (Q)
	144	phenylalanine (F)
35	145	valine (V)
	146	tryptophan (W)



In another embodiment, the site of one or more of the amino acid modifications occurs within about 10 angstroms from the  $\alpha$  carbon residue 54 of FimH. For example, residues 1, 2, 13, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 77, 78, 101, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143 and 144 of FimH (SEQ ID  
5 NO:3) (see Table 4)

Table 4: Residues 10 angstroms from the  $\alpha$  carbon of residue 54 in FimH

	residue position	wild type amino acid
10	1	phenylalanine (F)
	2	alanine (A)
	13	isoleucine (I)
	44	cysteine (C)
15	45	histidine (H)
	46	asparagine (N)
	47	aspartic acid (D)
	48	tyrosine (Y)
20	49	proline (P)
	50	glutamic acid (E)
	51	asparagine (N)
	52	isoleucine (I)
	53	threonine (T)
25	54	aspartic acid (D)
	55	tyrosine (Y)
	56	valine (V)
	57	threonine (T)
30	91	proline (P)
	92	arginine (R)
	93	valine (V)
	94	valine (V)
35	95	tyrosine (Y)



	96	asparagine (N)
	97	serine (S)
	98	arginine (R)
5	99	threonine (T)
	101	lysine (K)
	131	leucine (L)
	132	arginine (R)
10	133	glutamine (Q)
	134	threonine (T)
	135	asparagine (N)
	136	asparagine (N)
15	137	tyrosine (Y)
	138	asparagine (N)
	139	serine (S)
	140	aspartic acid (D)
20	141	aspartic acid (D)
	142	phenylalanine (F)
	143	glutamine (Q)
	144	phenylalanine (F)

25 In another embodiment, the site of one or more of the amino acid modifications occurs within about 5 angstroms from the  $\alpha$  carbon of residue 54 of FimH. For example, the modification is at one or more of residues 1, 45, 46, 47, 52, 53, 54, 55, 56, 93, 94, 95, 133, 134 and 135 of FimH (SEQ ID NO:3). (see Table 5)

30 Table 5: Residues 5 angstroms from the  $\alpha$  carbon of residue 54 in FimH

	<b>residue position</b>	<b>wild type amino acid</b>
	1	phenylalanine (F)
	45	histidine (H)
35	46	asparagine (N)



47	aspartic acid (D)
52	isoleucine (I)
53	threonine (T)
54	aspartic acid (D)
55	tyrosine (Y)
56	valine (V)
93	valine (V)
94	valine (V)
95	tyrosine (Y)
133	glutamine (Q)
134	threonine (T)
135	asparagine (N)

In another embodiment, the amino acid modifications are made within 15, 10 and 5 angstroms of the  $\alpha$ -carbon of residues 1, 13, 46, 47, 48, 54, 133, 135, 140 or 142 of the FimH binding domain.

## 5.2 PROPHYLACTIC AND THERAPEUTIC USES

The present invention encompasses methods of treatment and prophylaxis and therapies which involve administering mutant proteins or polypeptides to an animal, preferably a mammal, and most preferably a human, for preventing, treating, or ameliorating symptoms associated with a disease, disorder, or infection. Prophylactic and therapeutic compounds of the invention include, but are not limited to, mutant proteins, polypeptides, antibodies elicited by the mutant proteins and polypeptides and nucleic acids encoding the proteins and antibodies. Proteins and antibodies may be provided in pharmaceutically acceptable compositions as known in the art or as described herein.

Methods of the invention include methods of treatment and prophylaxis involving administration of a mutant polypeptide or protein of the invention that elicits high potency inhibitory antibodies that inhibit or reduce protein binding, particularly where the protein binding is relevant to some disease or disorder. For example, peptides which elicit antibodies and the resulting antibodies which disrupt or prevent the interaction between an antigen and its binding partner may be administered to an animal, preferably a mammal and



most preferably a human, to treat, prevent or ameliorate one or more symptoms associated with infection.

In a specific embodiment, the methods of the invention produce antibodies that prevent a viral or bacterial antigen from binding to its binding partner (e.g., host cell  
5 receptor) by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 40%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to antigen binding to its host cell receptor in the absence of said antibodies.

Peptides and proteins that elicit antibodies which do not prevent a viral or  
10 bacterial antigen from binding its host cell receptor but inhibit or downregulate viral or bacterial replication can also be administered to an animal to treat, prevent or ameliorate one or more symptoms associated with a viral or bacterial infection. The ability of an antibody to inhibit or downregulate viral or bacterial replication may be determined by techniques described herein or otherwise known in the art. For example, the inhibition or  
15 downregulation of viral replication can be determined by detecting the viral titer in the animal.

Examples of pathogen host cell receptor interactions that may be disrupted in methods of the invention include, but are not limited to, those in Table 6.

20 Table 6

Pathogen	Cellular Receptor
B-lymphotropic papovavirus (LAV)	LAV receptor on B-cells
25 Bordetella pertussis	Adenylate cyclase
Borna Disease virus (BDV)	BDV surface glycoproteins
Bovine coronavirus	N-acetyl-9-O-acetylneuraminic acid receptor
Choriomeningitis virus	CD4+
30 Dengue virus	Highly sulphated type Heparin sulphate p65
<i>E. coli</i>	Gal $\alpha$ (1-4)Gal-containing receptors mannose-containing receptors
Ebola	CD16b



Pathogen	Cellular Receptor
Echovirus 1	Integrin VLA-2 receptor
Echovirus-11 (EV)	EV receptor
5 Endotoxin (LPS)	CD14
Enteric bacteria	Glycoconjugate receptors
Enteric Orphan virus	alpha/beta T-cell receptor
Enteroviruses	Decay-accelerating factor receptor
10 Feline leukemia virus	Extracellular envelope glycoprotein (Env-SU) receptor
Foot and mouth disease virus	Immunoglobulin Fc receptorPoxvirusM-T7
Gibbon ape leukemia virus (GALV)	GALV receptor
15 Gram-negative bacteria	CD14 receptor
Helicobacter pylori	Lewis(b) blood group antigen receptor
Hepatitis B virus (HBV)	T-cell receptor
Herpes Simplex Virus	Heparin sulphate glycoaminoglycan receptor Fibroblast growth factor receptor
20 HIV-1	CC-Chemokine receptor CCR5 CD11a CD2 G-protein coupled receptor CD4
25 Human cytomegalovirus	Heparin sulphate proteoglycan Annexin II CD13 (aminopeptidase N)
Human coronavirus	Human aminopeptidase N receptor
30 Influenza A, B & C	Hemagglutinin receptor
35 Legionella	CR3 receptor Protein kinase receptor Galactose N-acetylgalactosamine (Gal/GalNAc)- inhibitable lectin receptor Chemokine receptor



Pathogen	Cellular Receptor
Leishmania mexicana	Annexin I
Listeria monocytogenes	ActA protein
Measles virus	CD46 receptor
Meningococcus	Meningococcal virulence associated Opa receptors
Morbilliviruses	CD46 receptor
Mouse hepatitis virus	Carcinoembryonic antigen family receptors Carcinoembryonic antigen family Bg1a receptor
Murine leukemia virus	Envelope glycoproteins
Murine gamma herpes virus	gamma interferon receptor
Murine retrovirus	Glycoprotein gp70 Rmc-1 receptor
Murine coronavirus mouse hepatitis virus	Carcinoembryonic antigen family receptors
Mycobacterium avium-M	Human Integrin receptor alpha v beta 3
Neisseria gonorrhoeae	Heparin sulphate proteoglycan receptor CD66 receptor Integrin receptor Membrane cofactor protein CD46 GM1 GM2 GM3 CD3 Ceramide
Newcastle disease virus	Hemagglutinin-neuraminidase protein Fusion protein
Parvovirus B19	Erythrocyte P antigen receptor
Plasmodium falciparum	CD36 receptor Glycophorin A receptor
Pox Virus	Interferon gamma receptor



Pathogen	Cellular Receptor
Pseudomonas	KDEL receptor
Rotavirus	Mucosal homing alpha4beta7 receptor
Samonella typhiurium	Epidermal growth factor receptor
Shigella	$\alpha 5\beta 1$ integrin protein
Streptococci	Nonglycosylated J774 receptor
T-helper cells type 1	Chemokine receptors including: CXCR1-4 CCR1-5 CXCR3 CCR5
T-cell lymphotropic virus 1	gp46 surface glycoprotein
Vaccinia virus	TNFRp55 receptor TNFRp75 receptor Soluble Interleukin-1 $\beta$ receptor

In a specific embodiment, an antibody inhibits or downregulates viral or bacterial replication by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 40%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to viral or bacterial replication in absence of said antibody.

Proteins and peptides that elicit antibodies and the resulting antibodies can also be used to prevent, inhibit or reduce the growth or metastasis of cancerous cells. In a specific embodiment, an antibody inhibits or reduces the growth or metastasis of cancerous cells by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 40%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to the growth or metastasis in absence of said antibody. Examples of cancers include, but are not limited to, leukemia (*e.g.*, acute leukemia such as acute lymphocytic leukemia and acute myelocytic leukemia), neoplasms, tumors (*e.g.*, fibrosarcoma, myxosarcoma, liposarcoma, chondrosarcoma, osteogenic sarcoma, chordoma, angiosarcoma, endotheliosarcoma, lymphangiosarcoma,



lymphangi endotheliosarcoma, synovioma, mesothelioma, Ewing's tumor, leiomyosarcoma, rhabdomyosarcoma, colon carcinoma, pancreatic cancer, breast cancer, ovarian cancer, prostate cancer, squamous cell carcinoma, basal cell carcinoma, adenocarcinoma, sweat gland carcinoma, sebaceous gland carcinoma, papillary carcinoma, papillary  
5 adenocarcinomas, cystadenocarcinoma, medullary carcinoma, bronchogenic carcinoma, renal cell carcinoma, hepatoma, bile duct carcinoma, choriocarcinoma, seminoma, embryonal carcinoma, Wilms' tumor, cervical cancer, testicular tumor, lung carcinoma, small cell lung carcinoma, bladder carcinoma, epithelial carcinoma, glioma, astrocytoma, medulloblastoma, craniopharyngioma, ependymoma, pinealoma, hemangioblastoma,  
10 acoustic neuroma, oligodendroglioma, meningioma, melanoma, neuroblastoma, and retinoblastoma), heavy chain disease, metastases, or any disease or disorder characterized by uncontrolled cell growth.

Proteins and peptides that elicit antibodies and antibodies can also be used to reduce the inflammation experienced by animals, particularly mammals, with inflammatory  
15 disorders. In a specific embodiment, an antibody reduces the inflammation in an animal by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 40%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to the inflammation in an animal in the not administered said protein, peptide or antibody. Examples of inflammatory  
20 disorders include, but are not limited to, rheumatoid arthritis and asthma.

Peptides, proteins and antibodies of the invention can also be used to prevent the rejection of transplants. Antibodies can also be used to prevent clot formation. Further, peptides and proteins that elicit antibodies and antibodies that function as agonists of the immune response can also be administered to an animal, preferably a mammal, and most  
25 preferably a human, to treat, prevent or ameliorate one or more symptoms associated with the disease, disorder, or infection.

The compositions of this invention may also be advantageously utilized in combination with other monoclonal or chimeric antibodies, or with lymphokines or hematopoietic growth factors (such as, *e.g.*, IL-2, IL-3, IL-7, and IL-9), which, for example,  
30 serve to increase the number or activity of effector cells which interact with the antibodies. The antibodies of this invention may also be advantageously utilized in combination with other monoclonal or chimeric antibodies, or with lymphokines or hematopoietic growth factors (such as, *e.g.*, IL-2, IL-3, IL-7, and IL-9), which, for example, serve to increase the immune response. The compositions of this invention may also be advantageously utilized  
35 in combination with one or more drugs used to treat a disease, disorder, or infection such as,



for example anti-cancer agents, anti-inflammatory agents anti-viral agents, or antibiotics. Examples of anti-cancer agents include, but are not limited to, isplatin, ifosfamide, paclitaxel, taxanes, topoisomerase I inhibitors (*e.g.*, CPT-11, topotecan, 9-AC, and GG-211), gemcitabine, cisplatin, doxinedria, vinorelbine, oxaliplatin, 5-fluorouracil (5-FU),  
5 leucovorin, vinorelbine, temodal, and taxol. Examples of anti-viral agents include, but are not limited to, cytokines (*e.g.*, IFN- $\alpha$ , IFN- $\beta$ , IFN- $\gamma$ ), inhibitors of reverse transcriptase (*e.g.*, AZT, 3TC, D4T, ddC, ddI, d4T, 3TC, adefovir, efavirenz, delavirdine, nevirapine, abacavir, and other dideoxynucleosides or dideoxyfluoronucleosides), inhibitors of viral mRNA capping, such as ribavirin, inhibitors of proteases such HIV protease inhibitors (*e.g.*,  
10 amprenavir, indinavir, nelfinavir, ritonavir, and saquinavir,), amphotericin B, castanospermine as an inhibitor of glycoprotein processing, inhibitors of neuraminidase such as influenza virus neuraminidase inhibitors (*e.g.*, zanamivir and oseltamivir), topoisomerase I inhibitors (*e.g.*, camptothecins and analogs thereof), amantadine, and rimantadine. Examples of anti-inflammatory agents include, but are not limited to, nonsteroidal  
15 anti-inflammatory drugs such as COX-2 inhibitors (*e.g.*, meloxicam, celecoxib, rofecoxib, flosulide, and SC-58635, and MK-966), ibuprofen and indomethacin, and steroids (*e.g.*, deflazacort, dexamethasone and methylprednisolone).

In a specific embodiment, antibodies administered to an animal are of a species origin or species reactivity that is the same species as that of the animal. Thus, in a  
20 preferred embodiment, human or humanized antibodies, or nucleic acids encoding human or human, are administered to a human patient for therapy or prophylaxis.

In a preferred embodiment, the present invention encompasses the administration of a mutant bacterial adhesin protein or fragment thereof, preferably associated with a pathogenic bacteria. The mutant bacterial adhesin protein is preferably a  
25 type 1 pilus polypeptide. Fragments of the bacterial adhesin protein containing, for example, all or an immunogenic portion of the mutant attachment domain (preferably, a portion that binds cell surface residues and/or mannose) of the protein may also be administered. Such bacterial adhesin proteins also include analogs, homologs and variants thereof, preferably that retain decrease binding activity. In other embodiments, the mutant  
30 bacterial adhesin proteins are provided as part of a complex, for example, with a bacterial chaperone protein, as detailed below.

In preferred embodiments, the methods of the invention encompass administration of a mutant FimH protein, including variants, derivatives, analogs and fragments thereof, preferably variants, derivatives, analogs and fragments that have  
35 decreased mannose binding activity and, preferably, are immunogenic. In one embodiment



of the present invention, recombinantly produced mutant FimH proteins (as well as functional analogs) from bacteria that produce type 1 pili are contemplated.

In additional preferred embodiments, the methods of the invention encompass administration of an antibody or antigen binding fragment thereof directed to the mutant proteins that have inhibitory functions with respect to the infective properties of the pathogen (*e.g.*, prevent binding of the pathogen to its cellular receptor). In one embodiment of the present invention, recombinantly produced antibodies are contemplated.

In preferred embodiments, the invention provides methods of treating or preventing a bacterial infection, particularly a urogenital tract infection, more particularly a UTI, caused by a gram negative bacterium of the family Enterobacteriaceae, especially *E. coli*. In other embodiments, the infection is caused by *Staphylococcus saprophyticus* or *Staphylococcus aureus*, *Klebsiella spp.*, *Proteus spp.*, *Serratia spp.*, or *Pseudomonas spp.* In an alternative embodiment, the infection is caused by infection with unusual organisms such as parasites, *e.g.*, *Echinococcus*, *Schistosoma haematobium* or *mansoni*, protozoa, *e.g.*, *Trichomonas*, yeast such as *Candida spp.*, *Blastomyces spp.*, or *Coccidioides immitis*, or acid-fast organisms such as *Mycobacterium tuberculosis*. In preferred embodiments, the infection to be treated or prevented using the methods of the invention is a UTI, a bladder infection, a kidney infection, pyelonephritis, cystitis, and asymptomatic bacteriuria.

In one embodiment, the primate is a human. In another embodiment, the human subject is susceptible to a recurrence of UTI due to having had a prior UTI, particularly having had two, three or even more UTIs in one year, or has a familial susceptibility, *e.g.*, genetic predisposition. In other embodiments, the human subject is pregnant and/or hospitalized, or is immuno-compromised due, for example, to a secondary disease, such as HIV or cancer, or having undergone therapies therefor, has an HIV infection or has a cancer, or is in remission therefrom. In a specific embodiment, the human subject has asymptomatic bactourea and, in particular embodiments, also is diabetic and/or is a pregnant woman. Reduced levels of IL-6 and/or IL-8 as compared to the normal levels of IL-6 and IL-8 in pregnant women have been correlated with difficulty in clearing urinary tract infections. Thus, the invention further includes treatment of pregnant women with reduced levels of IL-6 and/or IL-8. In another specific embodiment, the subject is at risk of developing end stage renal disease; accordingly, the invention further provides a method for preventing progression to end stage renal disease.

In a preferred embodiment, the compositions of the invention are administered parenterally, preferably via intramuscular, intravenous or subcutaneous injection; orally; transdermally; nasally; muscosally, including vaginally, rectally, buccally,



preferably the mucosal delivery is via a vaginal suppository; and finally via pulmonary delivery. Preferably, the compositions are not injected intraperitoneally.

The polypeptides and antibodies of the present invention may also be present in the form of a composition. Such compositions, where used for pharmaceutical purposes, will commonly have the polypeptide of the present invention suspended in a pharmacologically acceptable diluent or excipient, or they may be in lyophilized form. The methods of the invention encompass administering an effective amount of composition to elicit sufficient levels of antibodies, particularly IgGs, in serum and, preferably, in mucosal secretions, such as urine and/or genital secretions, to prevent bacterial infection, *e.g.*, to reduce the incidence of such bacterial infections, or to treat or ameliorate the symptoms of bacterial infection.

### 5.3 PHARMACEUTICAL FORMULATIONS AND ADMINISTRATION OF MUTANT PROTEINS

The mutant polypeptides and fragments thereof described herein are useful immunogens for preparing pharmaceutical compositions that stimulate the production of antibodies that inhibit the interaction of binding partners. This antibody inhibition is greater than that of antibodies raised against the corresponding non-mutant polypeptides.

The antibodies of the invention can be directed to any protein that has a binding partner. In preferred embodiments, the antibodies have enhanced functional inhibitory activity to block binding of a pathogenic protein to its host cell receptor. A particular embodiment of the invention provides antibodies having enhanced ability to block binding of a parasitic ligand to its host cell receptor. Highly preferred embodiments of the invention provide antibodies having enhanced ability to block binding of a microbial adhesin protein to its host cell receptor. In the most preferred embodiment, the microbial adhesion protein is FimH.

The pharmaceutical compositions useful herein also contain a pharmaceutically acceptable carrier, including any suitable diluent or excipient, which includes any pharmaceutical agent that does not itself induce the production of antibodies harmful to the primate receiving the composition, and which may be administered without undue toxicity.

In preferred embodiments, the pharmaceutical formulations of the invention comprise a FimH polypeptide (preferably, mutant FimH polypeptide of the invention), FimCH polypeptide complex (preferably where the FimH component is a mutant FimH of the invention) or fragments or variants thereof, and a pharmaceutically acceptable carrier or



excipient. Pharmaceutically acceptable carriers include but are not limited to saline, buffered saline, dextrose, water, glycerol, sterile isotonic aqueous buffer, and combinations thereof. A thorough discussion of pharmaceutically acceptable carriers, diluents, and other excipients is presented in *Remington's Pharmaceutical Sciences* (Mack Pub. Co., N.J. current edition). The formulation should suit the mode of administration. In a preferred embodiment, the formulation is suitable for administration to humans, preferably is sterile, non-particulate and/or non-pyrogenic. In a preferred embodiment the pharmaceutical composition contains a citrate buffer, preferably, about 20 mM sodium citrate and 0.2 M NaCl, more preferably with a pH of 6.0, and an adjuvant, such as MF59C.1 (Chiron, Emeryville, CA).

The composition, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents. The composition can be a solid form, such as a lyophilized powder suitable for reconstitution, a liquid solution, suspension, emulsion, tablet, pill, capsule, sustained release formulation, or powder. Oral formulation can include standard carriers such as pharmaceutical grades of mannitol, lactose, starch, magnesium stearate, sodium saccharine, cellulose, magnesium carbonate, etc.

Generally, the ingredients are supplied either separately or mixed together in unit dosage form, for example, as a dry lyophilized powder or water free concentrate in a hermetically sealed container such as an ampoule or sachette indicating the quantity of active agent. Where the composition is administered by injection, an ampoule of sterile diluent can be provided so that the ingredients may be mixed prior to administration.

The invention provides in one embodiment a thermally stable and/or chemically stable pharmaceutical composition that is suitable for reconstitution into an injectable sterile and particulate-free solution.

The invention also provides a pharmaceutical pack or kit comprising one or more containers filled with one or more of the ingredients of the vaccine formulations of the invention. In a preferred embodiment, the kit comprises two containers, one containing the adhesin protein or protein complex and the other containing an adjuvant. Associated with such container(s) can be a notice in the form prescribed by a governmental agency regulating the manufacture, use or sale of pharmaceuticals or biological products, which notice reflects approval by the agency of manufacture, use or sale for human administration.

The invention also provides that mutant polypeptide, or polypeptide complex or fragments thereof are packaged in a hermetically sealed container such as an ampoule or sachette indicating the quantity of composition. In one embodiment, the composition is supplied as a liquid, in another embodiment, as a dry sterilized lyophilized powder or water



free concentrate in a hermetically sealed container and can be reconstituted, e.g., with water or saline to the appropriate concentration for administration to a subject. Preferably, the composition is supplied as a dry sterile lyophilized powder in a hermetically sealed container at a unit dosage of preferably, 1  $\mu\text{g}$ , 5  $\mu\text{g}$ , 10  $\mu\text{g}$ , 20  $\mu\text{g}$ , 25  $\mu\text{g}$ , 30  $\mu\text{g}$ , 50  $\mu\text{g}$ , 75  $\mu\text{g}$ , 100  $\mu\text{g}$ , 123  $\mu\text{g}$ , 150  $\mu\text{g}$ , or 200  $\mu\text{g}$ . Alternatively, the unit dosage of the composition is less than 1  $\mu\text{g}$ , (for example 0.5  $\mu\text{g}$  or less, 0.25  $\mu\text{g}$  or less, or 0.1  $\mu\text{g}$  or less), or more than 123  $\mu\text{g}$ , (for example 150  $\mu\text{g}$  or more, 250  $\mu\text{g}$  or more, or 500  $\mu\text{g}$  or more).

The composition should be administered within 12 hours, preferably within 6 hours, within 5 hours, within 3 hours, or within 1 hour after being reconstituted from the lyophilized powder.

In an alternative embodiment, a mutant polypeptide or fragment thereof is supplied in liquid form in a hermetically sealed container indicating the quantity and concentration of the polypeptide composition. Preferably, the liquid form of the mutant polypeptide or fragment thereof is supplied in a hermetically sealed container at least 50  $\mu\text{g}/\text{ml}$ , more preferably at least 100  $\mu\text{g}/\text{ml}$ , at least 200  $\mu\text{g}/\text{ml}$ , at least 500  $\mu\text{g}/\text{ml}$ , at least 1  $\text{mg}/\text{ml}$ , and most preferably 490  $\mu\text{g}/\text{ml}$ .

In a preferred embodiment, mutant polypeptide is stored in a 3 ml sterile vial containing 1.0 ml of vaccine formulated in 500  $\mu\text{g}/\text{ml}$  of mutant polypeptide in 20 mM sodium citrate, 0.2 M NaCl at a pH of 6.0. In this formulation, the vial should contain a clear colorless liquid. The adjuvant is stored in a separate 3 ml vial containing 0.7 ml of adjuvant (MF59C.1; 39  $\text{mg}/\text{ml}$  squalene, 4.7  $\text{mg}/\text{ml}$  each Tween 80 and Span 85, 10 mM citrate in sterile water for injection at pH 6.5) and is typically a cloudy, white, turbid liquid. The diluent is supplied in another separate 3 ml vial containing 2.0 ml of 20 mM sodium citrate, 0.2 M NaCl at a pH of 6.0. The diluent is a clear, colorless liquid. Each of these vials should be stored in a refrigerator (2°C to 8°C/36°F to 46°C).

In a preferred embodiment, the mutant polypeptide is prepared for injection into a subject immediately prior to the injection, i.e., mixed with diluent and adjuvant.

Doses of 1  $\mu\text{g}$ , 5  $\mu\text{g}$ , 25  $\mu\text{g}$  and 123  $\mu\text{g}$  of mutant polypeptide are preferably prepared for administration as follows:

For a 1  $\mu\text{g}$  dose, gently invert several times one mutant polypeptide vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.5 ml from the vaccine vial into a 1.0 ml syringe and inject into a diluent vial. Immediately mix by gently swirling. Withdraw 0.5 ml using a new needle and inject into a second diluent vial. Immediately mix by gently swirling. Withdraw 0.5 ml using a new needle and inject into the third diluent vial. Immediately mix by gently



swirling. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial. Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 1  $\mu$ g of mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

For a 5  $\mu$ g dose, gently invert several times one vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.5 ml using a new needle and inject into a second diluent vial. Immediately mix by gently swirling. Withdraw 0.5 ml using a new needle and inject into the third diluent vial. Immediately mix by gently swirling. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial. Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 5  $\mu$ g of the mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

For a 25  $\mu$ g dose, gently invert several times one vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.5 ml using a new needle and inject into the third diluent vial. Immediately mix by gently swirling. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial. Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 25  $\mu$ g of the mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

For a 123  $\mu$ g dose, gently invert several times one vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial. Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new



needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 123  $\mu$ g of the mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

In another specific embodiment, 1, 5, 25 or 123  $\mu$ g of the mutant polypeptide in 0.5 ml of MF59C.1, as prepared above, is injected slowly, *i.e.*, 20 to 30 seconds, into the deltoid muscle of the upper arm of the subject at day 0, followed by a booster dose approximately one month, and a second booster, if necessary approximately 4-6 months, after the initial administration. The necessity of booster shots can be determined by measuring serum, urine or mucosal secretions for immunoglobulins specific to the polypeptide injected.

### 5.3.1 ADJUVANTS

The invention encompasses mutant proteins *e.g.*, FimH compositions, for use in vaccines administered in conjunction with adjuvants, wherein the adjuvants can be mixed (before or simultaneously upon injection) with the mutant polypeptide composition or alternatively the adjuvant is not mixed with the mutant polypeptide composition but is separately co-administered with the mutant polypeptide composition.

Mutant polypeptide compositions are administered with one or more adjuvants. In one embodiment, the mutant polypeptide composition is administered together with a mineral salt adjuvants or mineral salt gel adjuvant. Such mineral salt and mineral salt gel adjuvants include, but are not limited to, aluminum hydroxide (ALHYDROGEL, REHYDRAGEL), aluminum phosphate gel, aluminum hydroxyphosphate (ADJU-PHOS), and calcium phosphate.

In another embodiment, the mutant polypeptide composition is administered with an immunostimulatory adjuvant. Such class of adjuvants, include, but are not limited to, cytokines (*e.g.*, interleukin-2, interleukin-7, interleukin-12, granulocyte-macrophage colony stimulating factor (GM-CSF), interferon- $\gamma$ , interleukin-1 $\beta$  (IL-1 $\beta$ ), and IL-1 $\beta$  peptide or Sclavo Peptide), cytokine-containing liposomes, triterpenoid glycosides or saponins (*e.g.*, QuilA and QS-21, also sold under the trademark STIMULON, ISCOPREP), Muramyl Dipeptide (MDP) derivatives, such as N-acetyl-muramyl-L-threonyl-D-isoglutamine (Threonyl-MDP, sold under the trademark TERMURTIDE), GMDP, N-acetyl-nor-muramyl-L-alanyl-D-isoglutamine, N-acetylmuramyl-L-alanyl-D-isoglutaminyl-L-alanine-2-(1'-2'-dipalmitoyl-sn-glycero-3-hydroxyphosphoryloxy)-ethylamine, muramyl tripeptide



phosphatidylethanolamine (MTP-PE), unmethylated CpG dinucleotides and oligonucleotides, such as bacterial DNA and fragments thereof, LPS, monophosphoryl Lipid A (3D-MLA sold under the trademark MPL), and polyphosphazenes.

5 In another embodiment, the adjuvant used is a CpG adjuvant. Oligo-deoxynucleotides (ODN) containing unmethylated CpG dinucleotides within specific sequence contexts (CpG motifs) are detected, like bacterial or viral DNA, as a danger signal by the vertebrate immune system. CpG ODN synthesized with a nuclease-resistant phosphorothioate backbone have been shown to be a potent Th1-directed adjuvant in mice. In addition, an ODN with a TpC dinucleotide at the 5' end followed by three 6 mer CpG motifs (5'-GTCGTT-3') separated by TpT dinucleotides has shown high immunostimulatory activity for human, chimpanzee, and rhesus monkey leukocytes (Hartmann et al., 2000, J. Immun., 164: 1617-1624).

15 In another embodiment, suitable adjuvants include, but are not limited to: aluminum hydroxide, N-acetyl-muramyl-L-threonyl-D-isoglutamine (thr-MDP), -acetyl-nor-muramyl-L-alanyl-D-isoglutamine, N-acetylmuramyl-L-alanyl-D-isoglutaminyl-L-alanine-2-(1'-2'-dipalmitoyl-sn-glycero-3-hydroxyphosphoryloxy)-ethylamine.

20 In another embodiment, the adjuvant used is a particulate adjuvant, including, but not limited to, emulsions, e.g., squalene or squalene oil-in-water adjuvant formulations, such as SAF and MF59, e.g., prepared with block-copolymers, such as L-121 (polyoxypropylene/polyoxyethylene) sold under the trademark PLURONIC L-121, Liposomes, Virosomes, cochleates, and immune stimulating complex, which is sold under the trademark ISCOM. In a preferred embodiment, the adjuvant is MF59, MF59C or most preferably MF59C.1 (Chiron, Emeryville, CA) or a derivative thereof. Freund's Complete Adjuvant and Freund's Incomplete Adjuvant are also commonly used adjuvants in test animals, however these adjuvants are less preferred in primates, in particular for use in humans.

30 In another embodiment, a microparticulate adjuvant is used. Microparticulate adjuvants include, but are not limited to biodegradable and biocompatible polyesters, homo- and copolymers of lactic acid (PLA) and glycolic acid (PGA), poly(lactide-co-glycolides) (PLGA) microparticles, polymers that self-associate into particulates (poloxamer particles), soluble polymers (polyphosphazenes), and virus-like particles (VLPs) such as recombinant protein particulates, e.g., hepatitis B surface antigen (HbsAg).

35 Yet another class of adjuvants that may be used include mucosal adjuvants, including but not limited to heat-labile enterotoxin from *Escherichia coli* (LT), cholera holotoxin (CT) and cholera Toxin B Subunit (CTB) from *Vibrio cholerae*, mutant toxins



(e.g. LTK63 and LTR72), microparticles, and polymerized liposomes. Additional examples of mucous targeting adjuvants are *E. coli* mutant heat-labile toxin LT's with reduced toxicity, live attenuated organisms that bind M cells of the gastrointestinal tract, such as *V. cholera* and *Salmonella typhi*, *Mycobacterium bovis* (BCG), in addition to mucosal targeted  
5 particulate carriers such as phospholipid artificial membrane vesicles, copolymer microspheres, lipophilic immune-stimulating complexes and bacterial outer membrane protein preparations (proteosomes).

In other embodiments, any of the above classes of adjuvants may be used in combination with each other or with other adjuvants. For example, non-limiting examples  
10 of combination adjuvant preparations that can be used to administer the FimH compositions of the invention include liposomes containing immunostimulatory protein, cytokines, or T-cell and/or B-cell peptides, or microbes with or without entrapped IL-2 or microparticles containing enterotoxin. Other adjuvants known in the art are also included within the scope of the invention (*Vaccine Design: The Subunit and Adjuvant Approach*, Chap. 7, Michael F.  
15 Powell and Mark J. Newman (eds.), Plenum Press, New York, 1995, which is incorporated herein in its entirety).

The effectiveness of an adjuvant may be determined by measuring the induction of specific antibodies directed against the FimH composition formulated with the particular adjuvant. In a preferred embodiment, the adjuvant MF59C.1 is mixed with the  
20 vaccine composition, and MF59C.1 is at a dose of approximately 10 mg squalene, in 15 mM sodium citrate and 0.1 M NaCl.



### 5.3.2 VACCINE ADMINISTRATION

The invention provides methods of treatment, prophylaxis, and amelioration of one or more symptoms associated with pathogen infection by administering to a subject of an effective amount of a vaccine preparation comprising a protein of the invention or  
5 fragment thereof. The subject is preferably a mammal such as non-primate (*e.g.*, cows, pigs, horses, cats, dogs, rats etc.) and a primate (*e.g.*, monkey such as a cynomolgous monkey and a human). In a preferred embodiment, the subject is a human. In specific embodiments, the subject is a woman. The antibodies are particularly useful in women previously infected with UTI, pregnant women, and sexually active women. Finally, women previously infected  
10 with sexually transmitted diseases or otherwise at risk of UTI are recipients of the antibodies of the invention. In another embodiment, the subject is a diabetic, preferably a diabetic woman. In another embodiment, diabetic subjects can be vaccinated with WT FimCH.

Vaccines are generally administered parenterally using methods known in the art, however, many methods of administration may be used including but not limited to oral,  
15 intradermal, intramuscular, intravenous, subcutaneous, transdermal, intranasal routes, via pulmonary delivery, via suppository (*e.g.*, vaginal suppository), via scarification (scratching through the top layers of skin, *e.g.*, using a bifurcated needle). In a preferred embodiment, the vaccine is administered intramuscularly. In yet another embodiment, administration is not intraperitoneal due to the substantial risks of first pass hepatic removal of the  
20 polypeptides and also because of risk of infection and adhesions.

Various delivery vehicles are known and can be used to administer the mutant polypeptide compositions of the invention or fragments thereof, *e.g.*, encapsulation in liposomes, microparticles, microcapsules, recombinant cells capable of expressing the mutant polypeptide compositions, receptor-mediated endocytosis (see, *e.g.*, Wu and Wu,  
25 1987, *J. Biol. Chem.* 262:4429-4432), construction of a nucleic acid as part of a retroviral or other vector, for example, the pCGA139-1-1 vector as described herein which can be administered as a DNA vaccine or alternatively, the nucleic acid vector can be introduced into a host cell such that the host cell expresses and secretes the vaccine composition, *e.g.*, the mutant polypeptide complex, and the host cell is subsequently implanted into the subject  
30 contained within a membrane suitable for human implantation.

Methods of administering a polypeptide or fragment thereof, or pharmaceutical composition include, but are not limited to, parenteral administration (*e.g.*, intradermal, intramuscular, intravenous and subcutaneous), epidural, mucosal (*e.g.*, intranasal and oral or pulmonary routes or by vaginal suppositories), and topically. In a  
35 specific embodiment, compositions of the present invention or fragments thereof are



administered intramuscularly, intravenously, subcutaneously, or transdermally. The compositions may be administered by any convenient route, for example by infusion or bolus injection, by absorption through epithelial or mucocutaneous linings (e.g., oral mucous, colon, conjunctiva, nasopharynx, oropharynx, vagina, urethra, urinary bladder and intestinal mucosa, etc.) and may be administered together with other biologically active agents. Administration can be systemic or local.

In yet another embodiment, the vaccine composition is administered in such a manner as to target mucous tissues in order to elicit an immune response at the site of immunization. For example, mucosa tissues such as gut associated lymphoid tissue (GALT) can be targeted for immunization by using oral administration of compositions which contain adjuvants with particular mucosa targeting properties. Additional mucosal tissues can also be targeted, such as nasopharyngeal lymphoid tissue (NALT) and bronchial-associated lymphoid tissue (BALT) (Langermann, 1996, *Seminars in Gast. Dis.*, 7:12-18); Wizemann et al., 1999, *Emerging Inf. Dis.*, 5:395-403; Service, 1994, *Science*, 265:1522-1524).

In a specific embodiment, it may be desirable to administer the pharmaceutical compositions of the invention locally to the area in need of treatment; this may be achieved by, for example, and not by way of limitation, local infusion, by injection, or by means of an implant, said implant being of a porous, non-porous, or gelatinous material, including membranes, such as sialastic membranes, or fibers. Preferably, when administering an antibody of the invention or fragment thereof, care must be taken to use materials to which the FimH compositions does not absorb.

In another embodiment, the composition can be delivered in a vesicle, in particular a liposome (Langer, 1990, *Science* 249:1527-1533); Treat et al., 1989, in *Liposomes in the Therapy of Infectious Disease and Cancer*, Lopez-Berestein and Fidler (eds.), Liss, New York, pp. 353- 365; Lopez-Berestein, *ibid.*, pp. 3 17-327; see generally *ibid.*).

In yet another embodiment, the composition can be delivered in a controlled release system. In one embodiment, a pump may be used (Langer, *supra*; Sefton, 1987, *CRC Crit. Ref. Biomed. Eng.* 14:20; Buchwald et al., 1980, *Surgery* 88:507; Saudek et al., 1989, *N. Engl. J. Med.* 321:574). In another embodiment, polymeric materials can be used (e.g., *Medical Applications of Controlled Release*, 1974, Langer and Wise (eds.), CRC Pres., Boca Raton, Florida; *Controlled Drug Bioavailability, Drug Product Design and Performance*, 1984, Smolen and Ball (eds.), Wiley, New York; Ranger and Peppas, 1983, *J. Macromol. Sci. Rev. Macromol. Chem.* 23:61; Levy et al., 1985, *Science* 228:190; During et al., 1989,



*Ann. Neurol.* 25:351; Howard *et al.*, 1989, *J.Neurosurg.* 71:105); U.S. Patent No. 5,679,377; U.S. Patent No. 5,916,597; U.S. Patent No. 5,912,015; U.S. Patent No. 5,989,463; U.S. Patent No. 5,128,326; PCT Publication No. WO 99/15154; and PCT Publication No. WO 99/20253. In yet another embodiment, a controlled release system can  
5 be placed in proximity of the therapeutic target, *e.g.*, the urogenital tract, thus requiring only a fraction of the systemic dose (*e.g.*, Goodson, 1984, in *Medical Applications of Controlled Release*, *supra*, vol. 2, pp. 115-138).

Other controlled release systems are discussed in the review by Langer (1990, *Science* 249:1527-1533).

10 In a specific embodiment where the composition of the invention is a nucleic acid encoding a mutant polypeptide, a mutant polypeptide complex or a fragments thereof, the nucleic acid can be administered *in vivo* to promote expression of its encoded mutant polypeptide compositions, by constructing it as part of an appropriate nucleic acid expression vector and administering it so that it becomes intracellular, *e.g.*, by use of a  
15 retroviral vector (U.S. Patent No. 4,980,286), or by direct injection, or by use of microparticle bombardment (*e.g.*, a gene gun; Biolistic, Dupont), or coating with lipids or cell-surface receptors or transfecting agents, or by administering it in linkage to a homeobox- like peptide which is known to enter the nucleus (*e.g.*, Joliot *et al.*, 1991, *Proc. Natl. Acad. Sci. USA* 88:1864-1868), etc. Alternatively, a nucleic acid can be introduced  
20 intra-cellularly and incorporated within host cell DNA for expression by homologous recombination.

Accordingly, also provided by the invention is a method for vaccinating a primate against urogenital tract infection, which method comprises administering to the primate a purified nucleic acid containing a nucleotide sequence encoding a mutant peptide  
25 or peptide complex comprising a mutant type 1 pilin polypeptide associated with a bacterium that causes a urogenital tract infection, said nucleic acid being administered in an amount effective to produce immunoglobulin molecules that specifically bind the type 1 pilin attachment domain. Pharmaceutical compositions containing nucleic acids comprising nucleotide sequences encoding bacterial adhesin proteins, or fragments or complexes  
30 thereof, are also provided.

The dosage of the pharmaceutical formulation can be determined readily by the skilled artisan, for example, by first identifying doses effective to elicit a prophylactic or therapeutic immune response, *e.g.*, by measuring the serum titer of vaccine specific immunoglobulins or by measuring the inhibitory ratio of serum samples, or urine samples,  
35 or mucosal secretions. In particular, doses that result in serum endpoint titers of at least



1:800, at least 1:1600, or at least 1:3200 and/or, which have at least 50% binding inhibition of *E. coli* to bladder cells, upon sample dilutions of at least 1:50, at least 1:100, at least 1:200, at least 1:400, at least 1:800, at least 1:1600, or at least 1:3200, and most preferably at least 1:1600, or have detectable specific and, preferably inhibitory immunoglobulins in urine or mucosal secretions, as taught in Section 5.3.3, in an animal model, such as a Cynomolgus monkey, before identifying the optimal dosage in humans.

In preferred embodiments, a dose of the purified mutant FimCH complex of 1 µg, 5 µg, 10 µg, 20 µg, 30 µg, 50 µg, 75 µg, 100 µg, 123 µg, 150 µg, or 200 µg, or preferably 25 µg is administered. In other embodiments, the dosage is in the range of 0.25 µg to 1 µg, 1 µg to 5 µg, 1 µg to 10 µg, 1 µg to 20 µg, 1 µg to 50 µg, 1 µg to 75 µg, 1 µg to 100 µg, 1 µg to 150 µg, 1 µg to 200 µg, 5 µg to 10 µg, 10 µg to 15 µg, 10 µg to 20 µg, 15 µg to 25 µg, 20 µg to 30 µg, 30 µg to 50 µg, 25 µg to 75 µg, 50 µg to 100 µg, 75 µg to 125 µg, 50 µg to 125 µg, 50 µg to 200 µg, or 100 µg to 200 µg. For pediatric uses, a fractional dose of the pharmaceutical composition may be administered. For adult patients or patients with persistent infections, larger doses may also be used.

Vaccines of the invention may also be administered on a dosage schedule, for example, an initial administration of the vaccine composition with subsequent booster administrations. In particular embodiments, a second dose of the pharmaceutical composition is administered anywhere from two weeks to one year, preferably from one to six months, after the initial administration. Additionally, a third dose may be administered after the second dose and from three months to two years, or even longer, preferably 4 to 6 months, or 6 months to one year after the initial administration. The third dose may be optionally administered when no or low levels of specific immunoglobulins are detected in the serum and/or urine or mucosal secretions of the subject after the second dose. In a preferred embodiment, a second dose is administered approximately one month after the first administration and a third dose is administered approximately six months after the first administration. In another preferred embodiment, the second dose is administered six months after the first administration.

### 5.3.3 DETERMINATION OF VACCINE EFFICACY

Immunopotency of the pharmaceutical formulations can be determined by monitoring the immune response of a subject following immunization with a mutant protein composition, in particular the generation of immunoglobulins, particularly IgGs, which are detectable in the urine or mucosal secretions of the subject. Generation of a humoral response may be taken as an indication of a generalized immune response, other components



of which, particularly cell-mediated immunity, may be important for protection against certain disorders. The disorder is UTI in a preferred embodiment. Vaccine efficacy for other mutant proteins for other indications may be determined by analogous methods using skill in the art.

5           Subjects can include any primate including *Cynomolgus* monkeys, chimpanzees and human subjects in well controlled clinical settings. In addition, bacteria causing UTI can be used to induce infection in primates experimentally. However, since many primates are a protected species, the antibody response to a vaccine of the invention can first be studied in a number of smaller, less expensive animals, with the goal of finding  
10 one or two best candidate viruses or best combinations of viruses to use in primate efficacy studies. As one example, UTI vaccines of the invention may be tested first in mice for the ability to induce an antibody response to mutant bacterial adhesin polypeptides or polypeptide complexes and to protect against bacterial challenge.

15           The methods of introduction of the vaccine in the test subjects may include oral, intradermal, intramuscular, intravenous, subcutaneous, intranasal or any other standard routes of immunization.

          The immune response of the test subjects can be analyzed by various approaches such as: the reactivity of the resultant immune serum or urine or mucosal secretions to *E. coli* pilus, as assayed by known techniques, *e.g.*, enzyme linked  
20 immunosorbent assay (ELISA), immunoblots, radio-immunoprecipitations, etc.; or protection from UTI infections and/or attenuation of UTI symptoms in immunized hosts, for example, but not limited to, cystitis; or inhibition of binding of *E. coli* to cell surface residues, particularly mannose residues.

          Urine and mucosa samples may be taken from the test subject every one or  
25 two weeks, and serum analyzed for inhibitory antibodies to *E. coli* Type 1 pilus using, *e.g.*, a functional test for inhibitory activity such as measured by the ability to block binding of type 1 pilated bacteria (*E. coli* strain NU14) to transformed human bladder J82 cell line. The presence of antibodies specific for that particular mutant FimH may be assayed by ELISA using the mutant Fim CH for capture protein.

30           *Cynomolgus* monkeys (*Macaca fascicularis*) may be used to test for immunogenicity of FimH vaccine formulations of the invention. In a specific embodiment, monkeys each receive intramuscularly approximately 100 µg or other appropriate dose of the mutant adhesin in adjuvant. A control *Cynomolgus* monkey receives adjuvant alone. Blood is drawn weekly for 12 weeks, and serum is analyzed for functionally inhibitory antibodies  
35



to the adhesin. Urine and vaginal samples are taken to assess, by ELISA or other antibody detection tests, particularly IgG secretion.

Furthermore, the antibodies that are produced in response to the vaccine can be assessed for functional activity, *e.g.*, binding to the adhesin or inhibiting binding of type 1 pilin bacteria to urogenital tract cells.

A non-limiting example of a binding inhibition assay is as follows. Type 1 piliated NU14 *E. coli* are directly labeled with fluorescein isothiocyanate (FITC) and incubated with J82 bladder cells at a ratio of 250 bacteria/cell in the presence of preimmune or immunized serum and incubated for 30 minutes at 37° C. After multiple washes, samples are assayed by flow cytometry, and percent inhibition of bacterial binding to the cells is determined. The samples, such as serum samples, urine samples or vaginal wash samples, are diluted at 1:2, 1:4, 1:8, up to 1:3200 or more, and compared relative to preimmune samples from each subject, in order to identify an endpoint dilution where the binding inhibition is equal to or less than 50%. The binding ratio is defined as the ratio of the number of bacteria or the mean channel fluorescent (MCF) value which correlates with the number of bacteria (*e.g.* NU14) bound to a cell (*e.g.*, J82) in the presence of a diluted sample from an immunized subject, relative to the number of bacteria which bind a cell in the presence of preimmune sample from a non-immunized subject.

Another non-limiting example of a binding inhibition assay is as follows. Briefly, Immulon-4 plates (Dynex Technologies, Inc., Chantilly, VA ) are coated with 2.5 µg/ml (100 µl/well) of tri-mannose-BSA (V-Labs, Covington, LA). Type 1-piliated NU14 *E. coli* are added to each well, incubated at 37°C for 1 hour and after extensive washing, bound bacteria are detected with a 1:400 dilution of an anti-*E. coli*-HRP conjugated antibody (Biodesign, Kennebunk, ME). OD<sub>405</sub> readings of these samples establish the full signal values (FSV) for binding to trimannose (approximately 2.0). Additional samples are run in the presence of 1:50 dilutions of serum to assess inhibition, where percent inhibition equals the FSV - the sample value/FSV x 100. All samples are run in triplicate.

#### 5.4 PHARMACEUTICAL FORMULATIONS AND ADMINISTRATION OF ANTIBODIES

The present invention is directed to antibody-based therapies which involve administering antibodies of the invention or fragments thereof to a mammal, preferably a human, for preventing, treating, or ameliorating symptoms associated with an infection. Prophylactic and therapeutic compounds of the invention include, but are not limited to, antibodies of the invention (including fragments, analogs and derivatives thereof as



described herein) and nucleic acids encoding antibodies of the invention (including fragments, analogs and derivatives thereof and anti-idiotypic antibodies as described herein). Antibodies of the invention or fragments thereof may be provided in pharmaceutically acceptable compositions as known in the art or as described herein.

5           Antibodies of the present invention or fragments thereof that function as inhibitors of infection caused by a pathogen can be administered to a mammal, preferably a human, to treat, prevent or ameliorate one or more symptoms associated with infection. For example, antibodies or fragments thereof which disrupt or prevent the interaction between  
10 an antigen and its binding partner (*e.g.*, host cell receptor) may be administered to a mammal, preferably a human, to treat, prevent or ameliorate one or more symptoms associated with a infection.

          It is preferred to use high affinity and/or potent *in vivo* inhibiting antibodies and/or neutralizing antibodies that immunospecifically binds to a the pathogen antigen (*e.g.*, FimH), for prevention of infection and therapy for infection. It is also preferred to use  
15 polynucleotides encoding high affinity and/or potent *in vivo* inhibiting antibodies and/or neutralizing antibodies that immunospecifically bind to the pathogen antigen.

          In a specific embodiment, an antibody of the present invention or fragment thereof inhibits or decreases the pathogen's ability to infect a host by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at  
20 least 50%, at least 45%, at least 40%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to pathogen infection in absence of said antibodies or antibody fragments. In another embodiment, a combination of antibodies, a combination of antibody fragments, or a combination of antibodies and antibody fragments is used in the methods of the present invention. In a further embodiment, both the vaccines and antibodies  
25 can be used in combination to prevent, treat or manage disease or infection.

          One or more antibodies of the present invention or fragments thereof that immunospecifically bind to one or more pathogen mutant antigens may be used locally or systemically in the body as a therapeutic.

          In one embodiment, a mammal, preferably a human, is administered a first  
30 dose of a therapeutic or pharmaceutical composition comprising less than 15 mg/kg, preferably less than 10 mg/kg, less than 5 mg/kg, less than 3 mg/kg, less than 1 mg/kg or less than 0.5 mg/kg of one or more antibodies of the invention or fragments thereof for the prevention of an infection in an amount effective to induce a serum titer of at least 1 µg/ml, preferably at least 2 µg/ml, at least 5 µg/ml, at least 10 µg/ml, at least 15 µg/ml, at least 20  
35 µg/ml, or at least 25 µg/ml 20 days (preferably 25, 30, 35, 40 days) after the administration



of the first dose and prior to the administration of a subsequent dose. Preferably, the serum titer of said antibodies or antibody fragments is less than 30 µg/ml 30 days after the administration of the first dose and prior to the administration of a subsequent dose.

5 The present invention encompasses sustained release formulations comprising one or more antibodies or fragments thereof which have increased *in vivo* half-lives.

#### 5.4.1 METHODS OF ADMINISTRATION OF ANTIBODIES

10 The invention provides methods of treatment, prophylaxis, and amelioration of one or more symptoms associated with pathogen infection by administering to a subject of an effective amount of antibody or fragment thereof, or pharmaceutical composition comprising an antibody of the invention or fragment thereof. In a preferred aspect, an antibody or fragment thereof is substantially purified (*i.e.*, substantially free from substances that limit its effect or produce undesired side-effects). The subject is preferably a mammal  
15 such as non-primate (*e.g.*, cows, pigs, horses, cats, dogs, rats etc.) and a primate (*e.g.*, monkey such as a cynomolgous monkey and a human). In a preferred embodiment, the subject is a human. In specific embodiments, the subject is a woman. The antibodies are particularly useful in women previously infected with UTI, pregnant women and sexually active women. Finally, women previously infected with sexually transmitted diseases or  
20 otherwise at risk of UTI are recipients of the antibodies of the invention. In other embodiments, the subject is a diabetic, preferably a diabetic woman. In another embodiment, antibodies to WT FimCH can be administered to a diabetic subject.

Various delivery systems are known and can be used to administer an antibody of the invention or a fragment thereof, *e.g.*, encapsulation in liposomes,  
25 microparticles, microcapsules, recombinant cells capable of expressing the antibody or antibody fragment, receptor-mediated endocytosis (see, *e.g.*, Wu and Wu, 1987, *J. Biol. Chem.* 262:4429-4432), construction of a nucleic acid as part of a retroviral or other vector, etc. Methods of administering an antibody or fragment thereof, or pharmaceutical composition include, but are not limited to, parenteral administration (*e.g.*, intradermal,  
30 intramuscular, intraperitoneal, intravenous and subcutaneous), epidural, mucosal (*e.g.*, intranasal, vaginal, buccal and oral routes), oral and topical. In a specific embodiment, antibodies of the present invention or fragments thereof, or pharmaceutical compositions are administered intramuscularly, intravenously, or subcutaneously. The compositions may be administered by any convenient route, for example by infusion or bolus injection, by  
35 absorption through epithelial or mucocutaneous linings (*e.g.*, oral mucosa, rectal and



intestinal mucosa, etc.) and may be administered together with other biologically active agents. Administration can be systemic or local. In addition, pulmonary administration can also be employed, *e.g.*, by use of an inhaler or nebulizer, and formulation with an aerosolizing agent. See, *e.g.*, U.S. Patent Nos. 6,019,968, 5,985,320, 5,985,309, 5,934,272, 5,874,064, 5,855,913, 5,290,540, and 4,880,078, and PCT Publication Nos. WO 92/19244, WO 97/32572, WO 97/44013, WO 98/31346, and WO 99/66903, each of which is incorporated herein by reference their entirety.

The invention also provides that an antibody or fragment thereof is packaged in a hermetically sealed container such as an ampoule or sachette indicating the quantity of antibody or antibody fragment. In one embodiment, the antibody or antibody fragment is supplied as a dry sterilized lyophilized powder or water free concentrate in a hermetically sealed container and can be reconstituted, *e.g.*, with water or saline to the appropriate concentration for administration to a subject. Preferably, the antibody or antibody fragment is supplied as a dry sterile lyophilized powder in a hermetically sealed container at a unit dosage of at least 5 mg, more preferably at least 10 mg, at least 15 mg, at least 25 mg, at least 35 mg, at least 45 mg, at least 50 mg, or at least 75 mg. The lyophilized antibody or antibody fragment should be stored at between 2 and 8°C in its original container and the antibody or antibody fragment should be administered within 12 hours, preferably within 6 hours, within 5 hours, within 3 hours, or within 1 hour after being reconstituted. In an alternative embodiment, an antibody or fragment thereof is supplied in liquid form in a hermetically sealed container indicating the quantity and concentration of the antibody or antibody fragment. Preferably, the liquid form of the antibody or fragment thereof is supplied in a hermetically sealed container at least 1 mg/ml, more preferably at least 2.5 mg/ml, at least 5 mg/ml, at least 8 mg/ml, at least 10 mg/ml, at least 15 mg/kg, or at least 25 mg/ml.

In a specific embodiment, it may be desirable to administer the pharmaceutical compositions of the invention locally to the area in need of treatment; this may be achieved by, for example, and not by way of limitation, local topical administration, local infusion, by injection, or by means of an implant, said implant being of a porous, non-porous, or gelatinous material, including membranes, such as sialastic membranes, or fibers. Preferably, when administering a an antibody of the invention or fragment thereof, care must be taken to use materials to which the antibody or antibody fragment does not absorb.

In another embodiment, the composition can be delivered in a vesicle, in particular a liposome (see Langer, 1990, *Science* 249:1527-1533; Treat *et al.*, 1989, in



Liposomes in the Therapy of Infectious Disease and Cancer, Lopez-Berestein and Fidler (eds.), Liss, New York, pp. 353- 365; Lopez-Berestein, *ibid.*, pp. 3 17-327; see generally *ibid.*).

5 In yet another embodiment, the composition can be delivered in a controlled release system. In one embodiment, a pump may be used (see Langer, *supra*; Sefton, 1987, CRC Crit. Ref. Biomed. Eng. 14:20; Buchwald *et al.*, 1980, Surgery 88:507; Saudek *et al.*, 1989, N. Engl. J. Med. 321:574). In another embodiment, polymeric materials can be used to achieve controlled release of the antibodies of the invention or fragments thereof (see *e.g.*, Medical Applications of Controlled Release, Langer and Wise (eds.), CRC Pres., Boca  
10 Raton, Florida (1974); Controlled Drug Bioavailability, Drug Product Design and Performance, Smolen and Ball (eds.), Wiley, New York (1984); Ranger and Peppas, 1983, J., Macromol. Sci. Rev. Macromol. Chem. 23:61; see also Levy *et al.*, 1985, Science 228:190; During *et al.*, 1989, Ann. Neurol. 25:351; Howard *et al.*, 1989, J. Neurosurg. 7 1:105); U.S. Patent No. 5,679,377; U.S. Patent No. 5,916,597; U.S. Patent No. 5,912,015;  
15 U.S. Patent No. 5,989,463 ; U.S. Patent No. 5,128,326; PCT Publication No. WO 99/15154; and PCT Publication No. WO 99/20253. In yet another embodiment, a controlled release system can be placed in proximity of the therapeutic target, *i.e.*, the lungs, thus requiring only a fraction of the systemic dose (see, *e.g.*, Goodson, in Medical Applications of Controlled Release, *supra*, vol. 2, pp. 115-138 (1984)).

20 Other controlled release systems are discussed in the review by Langer (1990, Science 249:1527-1533).

In yet another embodiment, compositions comprising antibodies of the invention or fragments thereof are formulated for sustained release. Any technique known to one of skill in the art can be used to produce sustained release formulations comprising  
25 one or more antibodies of the invention or fragments thereof. See, *e.g.*, U.S. Patent No. 4,526,938, PCT publication WO 91/05548, PCT publication WO 96/20698, Ning *et al.*, 1996, "Intratumoral Radioimmunotherapy of a Human Colon Cancer Xenograft Using a Sustained-Release Gel," Radiotherapy & Oncology 39:179-189, Song *et al.*, 1995, "Antibody Mediated Lung Targeting of Long-Circulating Emulsions," PDA Journal of  
30 Pharmaceutical Science & Technology 50:372-397, Cleek *et al.*, 1997, "Biodegradable Polymeric Carriers for a bFGF Antibody for Cardiovascular Application," Pro. Int'l. Symp. Control. Rel. Bioact. Mater. 24:853-854, and Lam *et al.*, 1997, "Microencapsulation of Recombinant Humanized Monoclonal Antibody for Local Delivery," Proc. Int'l. Symp. Control Rel. Bioact. Mater. 24:759-760, each of which is incorporated herein by reference in  
35 their entirety.



In a specific embodiment where the composition of the invention is a nucleic acid encoding an antibody or antibody fragment, the nucleic acid can be administered *in vivo* to promote expression of its encoded antibody or antibody fragment, by constructing it as part of an appropriate nucleic acid expression vector and administering it so that it becomes  
5 intracellular, *e.g.*, by use of a retroviral vector (see U.S. Patent No. 4,980,286), or by direct injection, or by use of microparticle bombardment (*e.g.*, a gene gun; Biolistic, Dupont), or coating with lipids or cell-surface receptors or transfecting agents, or by administering it in linkage to a homeobox-like peptide which is known to enter the nucleus (*see e.g.*, Joliot *et al.*, 1991, *Proc. Natl. Acad. Sci. USA* 88:1864-1868), etc. Alternatively, a nucleic acid can  
10 be introduced intracellularly and incorporated within host cell DNA for expression by homologous recombination.

The present invention also provides pharmaceutical compositions. Such compositions comprise a prophylactically or therapeutically effective amount of an antibody or a fragment thereof, and a pharmaceutically acceptable carrier. In a specific embodiment,  
15 the term "pharmaceutically acceptable" means approved by a regulatory agency of the Federal or a state government or listed in the U.S. Pharmacopeia or other generally recognized pharmacopeia for use in animals, and more particularly in humans. The term "carrier" refers to a diluent, adjuvant (*e.g.*, Freund's adjuvant (complete and incomplete)), excipient, or vehicle with which the therapeutic is administered. Such pharmaceutical  
20 carriers can be sterile liquids, such as water and oils, including those of petroleum, animal, vegetable or synthetic origin, such as peanut oil, soybean oil, mineral oil, sesame oil and the like. Water is a preferred carrier when the pharmaceutical composition is administered intravenously. Saline solutions and aqueous dextrose and glycerol solutions can also be employed as liquid carriers, particularly for injectable solutions. Suitable pharmaceutical  
25 excipients include starch, glucose, lactose, sucrose, gelatin, malt, rice, flour, chalk, silica gel, sodium stearate, glycerol monostearate, talc, sodium chloride, dried skim milk, glycerol, propylene, glycol, water, ethanol and the like. The composition, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents. These compositions can take the form of solutions, suspensions, emulsion, tablets, pills, capsules,  
30 powders, sustained-release formulations and the like. Oral formulation can include standard carriers such as pharmaceutical grades of mannitol, lactose, starch, magnesium stearate, sodium saccharine, cellulose, magnesium carbonate, etc. Examples of suitable pharmaceutical carriers are described in "Remington's Pharmaceutical Sciences" by E.W. Martin. Such compositions will contain a prophylactically or therapeutically effective  
35 amount of the antibody or fragment thereof, preferably in purified form, together with a



suitable amount of carrier so as to provide the form for proper administration to the patient. The formulation should suit the mode of administration.

5 In a preferred embodiment, the composition is formulated in accordance with routine procedures as a pharmaceutical composition adapted for intravenous administration to human beings. Typically, compositions for intravenous administration are solutions in sterile isotonic aqueous buffer. Where necessary, the composition may also include a solubilizing agent and a local anesthetic such as lignocaine to ease pain at the site of the injection.

10 Generally, the ingredients of compositions of the invention are supplied either separately or mixed together in unit dosage form, for example, as a dry lyophilized powder or water free concentrate in a hermetically sealed container such as an ampoule or sachette indicating the quantity of active agent. Where the composition is to be administered by infusion, it can be dispensed with an infusion bottle containing sterile pharmaceutical grade water or saline. Where the composition is administered by injection, 15 an ampoule of sterile water for injection or saline can be provided so that the ingredients may be mixed prior to administration.

The compositions of the invention can be formulated as neutral or salt forms. Pharmaceutically acceptable salts include those formed with anions such as those derived from hydrochloric, phosphoric, acetic, oxalic, tartaric acids, etc., and those formed with 20 cations such as those derived from sodium, potassium, ammonium, calcium, ferric hydroxides, isopropylamine, triethylamine, 2-ethylamino ethanol, histidine, procaine, etc.

### 5.5 RECOMBINANT NUCLEIC ACIDS

25 Nucleic acid sequences changes can be introduced by mutation thereby leading to changes in the amino acid sequence of the encoded protein. For example, one can make nucleotide substitutions leading to amino acid substitutions at "non-essential" amino acid residues. A "non-essential" amino acid residue is a residue that can be altered from the wild-type sequence without altering the biological activity, whereas an "essential" amino acid residue is required for biological activity. For example, amino acid residues that are not 30 conserved or only semi-conserved among homologous of various species may be non-essential for activity and thus would be likely targets for alteration. Alternatively, amino acid residues that are conserved among the homologous of various species (e.g., murine and human) may be essential for activity and thus would not be likely targets for alteration.

35 Accordingly, another aspect of the invention pertains to nucleic acid molecules encoding a polypeptide of the invention that contain changes in amino acid



residues. Such polypeptides differ in amino acid sequence from wild type protein. In one embodiment, the domain which interacts with the wild type protein's binding partner is mutated. For example, in the bacterial adhesin FimH, amino acid substitutions can be introduced into residues listed in Section 5.1 above.

5           An isolated nucleic acid molecule encoding a variant protein can be created by introducing one or more nucleotide substitutions, additions or deletions into the nucleotide sequence, such that one or more amino acid substitutions, additions or deletions are introduced into the encoded protein. Mutations can be introduced by standard techniques, such as site-directed mutagenesis and PCR-mediated mutagenesis. Briefly, PCR  
10 primers are designed that delete the trinucleotide codon of the amino acid to be changed and replace it with the trinucleotide codon of the amino acid to be included. This primer is used in the PCR amplification of DNA encoding the protein of interest. This fragment is then isolated and inserted into the full length cDNA encoding the protein of interest and expressed recombinantly. The resulting protein now includes the amino acid replacement.

15           Preferably, non-conservative amino acid substitutions are made at one or more amino acid residues. Non-conservative replacements are those that take place between families of amino acids that are unrelated in their side chains. Genetically encoded amino acids can be divided into four families: (1) acidic = aspartate, glutamate; (2) basic = lysine, arginine, histidine; (3) nonpolar = alanine, valine, leucine, isoleucine, proline,  
20 phenylalanine, methionine, tryptophan; and (4) uncharged polar = glycine, asparagine, glutamine, cysteine, serine, threonine, tyrosine. In similar fashion, the amino acid repertoire can be grouped as (1) acidic = aspartate, glutamate; (2) basic = lysine, arginine histidine, (3) aliphatic = glycine, alanine, valine, leucine, isoleucine, serine, threonine, with serine and threonine optionally be grouped separately as aliphatic-hydroxyl; (4) aromatic =  
25 phenylalanine, tyrosine, tryptophan; (5) amide = asparagine, glutamine; and (6) sulfur - containing = cysteine and methionine. (See, for example, Biochemistry, 4th ed., Ed. by L. Stryer, WH Freeman and Co.: 1995).

          Alternatively, mutations can be introduced randomly along all or part of the coding sequence, such as by saturation mutagenesis.

30           Mutagenesis may be performed in accordance with any of the techniques known in the art including, but not limited to, synthesizing an oligonucleotide having one or more modifications within the sequence to be modified. Site-specific mutagenesis allows the production of mutants through the use of specific oligonucleotide sequences which encode the DNA sequence of the desired mutation, as well as a sufficient number of adjacent  
35 nucleotides, to provide a primer sequence of sufficient size and sequence complexity to form



a stable duplex on both sides of the deletion junction being traversed. Typically, a primer of about 17 to about 75 nucleotides or more in length is preferred, with about 10 to about 25 or more residues on both sides of the junction of the sequence being altered. A number of such primers introducing a variety of different mutations at one or more positions may be used to generated a library of mutants.

The technique of site-specific mutagenesis is well known in the art, as exemplified by various publications (see, e.g., Kunkel *et al.*, *Methods Enzymol.*, 154:367-82, 1987, which is hereby incorporated by reference in its entirety). In general, site-directed mutagenesis is performed by first obtaining a single-stranded vector or melting apart of two strands of a double stranded vector which includes within its sequence a DNA sequence which encodes the desired peptide. An oligonucleotide primer bearing the desired mutated sequence is prepared, generally synthetically. This primer is then annealed with the single-stranded vector, and subjected to DNA polymerizing enzymes such as T7 DNA polymerase, in order to complete the synthesis of the mutation-bearing strand. Thus, a heteroduplex is formed wherein one strand encodes the original non-mutated sequence and the second strand bears the desired mutation. This heteroduplex vector is then used to transform or transfect appropriate cells, such as *E. coli* cells, and clones are selected which include recombinant vectors bearing the mutated sequence arrangement. As will be appreciated, the technique typically employs a phage vector which exists in both a single stranded and double stranded form. Typical vectors useful in site-directed mutagenesis include vectors such as the M13 phage. These phage are readily commercially available and their use is generally well known to those skilled in the art. Double stranded plasmids are also routinely employed in site directed mutagenesis which eliminates the step of transferring the gene of interest from a plasmid to a phage.

Alternatively, the use of PCR<sup>TM</sup> with commercially available thermostable enzymes such as *Taq* DNA polymerase may be used to incorporate a mutagenic oligonucleotide primer into an amplified DNA fragment that can then be cloned into an appropriate cloning or expression vector. See, e.g., Tomic *et al.*, 1987, *Nucleic Acids Res.*, 18:1656; Upender *et al.*, 1995, *BioTechniques*, 18:29-30, 32, 1995, for PCR<sup>TM</sup>-mediated mutagenesis procedures, which are hereby incorporated in their entireties. PCR<sup>TM</sup> employing a thermostable ligase in addition to a thermostable polymerase may also be used to incorporate a phosphorylated mutagenic oligonucleotide into an amplified DNA fragment that may then be cloned into an appropriate cloning or expression vector (see e.g., Michael, 1994, *BioTechniques*, 16:410-2, which is hereby incorporated by reference in its entirety).



Following mutagenesis, the encoded protein can be expressed recombinantly and the activity of the protein can be determined. Those showing desired activity can then be further characterized. In the present invention, mutant proteins which lose or have decreased biological activity (*e.g.*, binding) are of particular interest.

5

### 5.6 PROTEIN EXPRESSION AND PURIFICATION

The mutant adhesin proteins, complexes and fragments thereof (preferably mutant FimH proteins and polypeptides) maybe produced by any method available in the art. Those skilled in the art will readily be able to purify such proteins, fragments or complexes by routine techniques.

10

One problem with utilizing such proteins has been that synthesis of the polypeptide, such as FimH, results in a protein that falls short of attaining its native *in vivo* structure. Thus, there is a difference between the *in vivo* conformation of such a protein and that attained by a purified recombinant form of such protein. The reason for this difference in conformation has been determined. In general, a pilin protein, such as an adhesin like FimH, has a native conformation that is at least partly determined by the *in vivo* interaction of such protein with an additional protein, here a periplasmic chaperone protein called FimC. The resulting FimC-FimH (or FimCH) complex is the form that presents the native FimH conformation as seen *in vivo* and thus by the immune system (Choudhury *et al.*, 1999, *Science* 285, 1061; Sauer *et al.*, 1999, *Science* 285:1058). Consequently, the methods and compositions of the invention include such complexes where said proteins are co-expressed, or otherwise formed in a combined state, with their respective periplasmic chaperone thereby yielding the native complex normally seen *in vivo* by the immune system following infection by a disease causing pathogen. Accordingly, the present invention further encompasses administration of such pilin complexes, *i.e.*, complexes of FimC with a FimH polypeptide.

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FimH complexes can be readily produced by recombinant methods in such a way as to incorporate therein the sequences provided by FimC in the FimCH complex, thus yielding a native structure for FimH, which structure is immunogenic in nature. In essence, the portion of the FimC molecule that binds to FimH and directs its native conformation is engineered into the FimH structure itself, at the appropriate location, to result in a native FimH structure. This portion of the FimC molecule that binds to FimH in the FimCH complex is called a "donor strand" and the mechanism of formation of the native FimH structure using only this additional strand from FimC has been referred to as "donor strand complementation." Thus, the FimH complexes, can be produced in their "donor

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complemented" form to provide highly immunogenic structures for use in therapeutically effective vaccine compositions within the present invention. Such donor strand complemented forms are disclosed in detail in U.S. Application No. 09/615,846, filed July 13, 2000 and PCT/US00/19066, filed July 13, 2000, both entitled "Donor Strand  
5 Complemented Pilus-Based Vaccines", each of which is hereby incorporated by reference herein in its entirety.

Accordingly, in preferred embodiments, complexes of FimH and FimC are administered in the methods of the invention. Such complexes include FimH-FimC fusion proteins and complexes, preferably, containing an equimolar ratio of FimH and FimC. Any  
10 known FimC protein can be used in such complexes. Preferably the FimC protein is from the *E. coli* J96 isolate and has an amino acid sequence of Figure 1. In a more preferred embodiment, a FimCH complex containing a FimH protein and a FimC protein in equimolar amounts is administered, preferably where the FimH protein has an amino acid sequence (with one or more amino acid modifications, as discussed above) of Figure 1 and the FimC  
15 protein has an amino acid sequence of Figure 1. As described *infra*, the FimCH complexes can be expressed from the same plasmid, preferably under the control of separate promoters, and isolated from the host cell, *e.g.*, an *E. coli* host cell.

Complexes comprising the *E. coli* chaperone FimC and a FimH variant of the invention may be formed by co-expressing a FimH variant polypeptide, whose amino acid  
20 and nucleotide sequences are known in the art (such as the FimH having the amino acid sequence of Figure 1) along with a FimC variant polypeptide, whose amino acid and nucleotide sequences are known in the art (such as the FimC having the amino acid sequence of Figure 1), from a recombinant cell.

In addition, the FimC-mutant FimH complexes useful in vaccines can be  
25 recovered from the periplasmic spaces of cells of the indicated strains disclosed herein. These complexes are found in relatively large amounts in recombinant *E. coli* strains which express the FimC protein at levels in excess of those produced in wild type strains. A suitable recombinant strain is C600/pHJ9205, in which expression of FimC has been put under control of the arabinose promoter. Those skilled in the art will recognize that other  
30 promoter sequences that can be regulated easily may also be used. Of course, such cells are readily engineered to express one or more of the FimH variant polypeptides of the invention. An extract of periplasm is obtained by exposing the bacteria to lysozyme in the presence of a hypertonic sucrose solution. FimCH complexes can also be purified using conventional  
35 protein purification methods well known in the art.



In a similar manner, FimH fragments can be recombinantly produced either by having *E. coli* produce the full-length FimH and then fragmenting the protein or may be isolated by mannose-binding affinity purification. Thus, only fragments of the FimH protein that retain mannose binding are isolated. Preferably, such mannose-binding fragments have a label such as a his-tag included and may be purified by methods such as nickel chromatography.

In accordance with the foregoing, FimC of *E. coli* is available through the American Type Culture Collection (ATCC) as accession number Z37500. A FimH protein of *E. coli* is available as ATCC Accession No. 1361011.

The polynucleotides encoding the mutant protein or polypeptide above may have the coding sequence fused in frame to a marker sequence which allows for purification of the polypeptides of the present invention. The marker sequence may be, for example, a hexa-histidine tag supplied by a pQE-9 vector to provide for purification of the mature polypeptides fused to the marker in the case of a bacterial host, or, for example, the marker sequence may be a hemagglutinin (HA) tag when a mammalian host, *e.g.* COS-7 cells, is used. The HA tag corresponds to an epitope derived from the influenza hemagglutinin protein (Wilson, *et al.*, 1984, *Cell*, 37:767).

The proteins and polypeptide of the invention may be recombinantly produced in an *E. coli* species host. Mutant FimH may likewise be produced recombinantly by producing the appropriate donor strand complemented version of FimH, wherein the amino acid sequence of FimC that interacts with mutant FimH in the FimCH complex is itself engineered at the C-terminal end of mutant FimH to provide the native conformation without the need for the remainder of the FimC molecule to be present. Additionally, mutant FimH variants may also be utilized in the form of a complex comprising isolated domains thereof, especially mannose-binding domains and fragments, which domains or fragments may be linked together, either covalently or non-covalently, utilizing linking segments, such linking segments being formed of amino acid sequences or other oligomeric structures, including simple polymer structures, to provide an overall structure exhibiting immunogenic activity.

In producing said proteins, particularly the adhesin protein recombinantly, a preferred host is a species of bacteria that can be cultured under conditions such that the usher gene (if present) is not expressed. Further preferred is a host species that is missing the usher gene or has a defective usher gene. Even further preferred is a host which is missing the pilus proteins other than the FimH protein (and may also produce the chaperone, such as FimC). When an adhesin protein or a mannose binding fragment of such adhesin



protein is to be produced in the absence of its chaperone protein (or to be separated from the chaperone after production), the mutant adhesin protein (or fragment) may be permitted to become properly folded in the presence of its chaperone protein and is then separated from the chaperone protein.

5           The present invention also relates to vectors which include polynucleotides encoding one or more of the mutant protein or polypeptides of the present invention, host cells which are genetically engineered with vectors of the invention, including host cells containing a nucleotide sequence encoding a protein of the invention operably linked to a heterologous promoter, and the production of such mutant adhesin proteins and/or  
10       chaperone proteins by recombinant techniques in an isolated and substantially immunogenically pure form.

          Host cells are genetically engineered (transduced or transformed or transfected) with the vectors comprising a polynucleotide encoding a chaperone, mutant  
15       adhesin protein, or the like, which may be, for example, a cloning vector or an expression vector. The vector may be, for example, in the form of a plasmid, a viral particle, a phage, etc. The engineered host cells can be cultured in conventional nutrient media modified as appropriate for activating promoters, selecting transformants or amplifying the  
polynucleotides which encode such polypeptides. The culture conditions, such as  
temperature, pH and the like, are those previously used with the host cell selected for  
20       expression, and will be apparent to the ordinarily skilled artisan.

          Vectors include chromosomal, nonchromosomal and synthetic DNA  
sequences, *e.g.*, derivatives of SV40; bacterial plasmids; phage DNA; baculovirus; yeast  
plasmids; vectors derived from combinations of plasmids and phage DNA, viral DNA such  
as retrovirus, vaccinia, adenovirus, fowl pox virus, and pseudorabies. However, any other  
25       vector may be used as long as it is replicable and viable in the host.

          The appropriate DNA sequence may be inserted into the vector by a variety  
of procedures. In general, the DNA sequence is inserted into an appropriate restriction  
endonuclease site(s) by procedures known in the art. Such procedures and others are  
deemed to be within the scope of those skilled in the art.

30           The DNA sequence in the expression vector is operatively linked to an appropriate expression control sequence(s) (promoter) to direct mRNA synthesis. As representative examples of such promoters, there may be mentioned: LTR or SV40 promoter, the *E. coli. lac* or *trp*, the phage lambda P<sub>L</sub> promoter and other promoters known  
to control expression of genes in prokaryotic or eukaryotic cells or their viruses. The  
35       expression vector also contains a ribosome binding site for translation initiation and a



transcription terminator. The vector may also include appropriate sequences for amplifying expression.

In addition, the expression vectors preferably contain one or more selectable marker genes to provide a phenotypic trait for selection of transformed host cells such as dihydrofolate reductase or neomycin resistance for eukaryotic cell culture, or such as tetracycline or ampicillin resistance in prokaryotic cell culture, *e.g.*, *E. coli*.

Optimal expression of a wild type FimCH complex has been achieved using a newly constructed single vector containing the FimH and FimC genes but having the advantage that each gene is under its own separate lac promoter. Thus, one lac promoter is 5' with respect to FimC while the second lac promoter is 5' to the FimH gene. This plasmid was successfully constructed using the common plasmid pUC19 as a background vector (Yannish-Perron, *et al.*, 1985, *Gene*, 33:103-119). This new plasmid, when used to transform the host *E. coli* strain BL21 (as described in Phillips, *et al.*, 1984, *J. Bacteriol.* 159:283-287) and then induced using IPTG at the mid-logarithmic stage of growth, gives maximal expression of the FimCH complex in the bacterial periplasmic space. This material is then extracted and purified by methods well known in the art, including those described herein. Such a plasmid can be constructed that encodes a wild type FimC in combination with a mutant FimH.

The vector containing the appropriate DNA sequence as hereinabove described, as well as an appropriate promoter or control sequence, may be employed to transform an appropriate host to permit the host to express the proteins.

As representative examples of appropriate hosts, there may be mentioned: bacterial cells, such as *E. coli*, *Streptomyces*, *Salmonella typhimurium*; fungal cells, such as yeast; insect cells such as *Drosophila* S2 and *Spodoptera* Sf9; animal cells such as CHO, COS or Bowes melanoma; adenoviruses; plant cells, etc. The selection of an appropriate host is deemed to be within the scope of those skilled in the art from the teachings herein.

Constructs for production of the adhesin proteins comprise a vector, such as a plasmid or viral vector, into which a sequence of the invention has been inserted, in a forward or reverse orientation. The construct may further comprise regulatory sequences, including, for example, a promoter, operably linked to the sequence. Large numbers of suitable vectors and promoters are known to those of skill in the art, and are commercially available. The following vectors are provided by way of example. Bacterial: pQE70, pQE60, pQE-9 (Qiagen, Inc.), pbs, pD10, phagescript, psiX174, pbluescript SK, pbsks, pNH8A, pNH16a, pNH18A, pNH46A (Stratagene); ptrc99a, pKK223-3, pKK233-3, pDR540, pRIT5 (Pharmacia). Eukaryotic: pWLNEO, pSV2CAT, pOG44, pXT1, pSG



(Stratagene) pSVK3, pBPV, pMSG, pSVL (Pharmacia). However, any other plasmid or vector may be used as long as they are replicable and viable in the host.

Promoter regions can be selected from any desired gene using CAT (chloramphenicol transferase) vectors or other vectors with selectable markers. Two  
5 appropriate vectors are pKK232-8 and pCM7. Particular named bacterial promoters include lacI, lacZ, T3, T7, gpt, lambda P<sub>R</sub>, P<sub>L</sub> and TRP. Eukaryotic promoters include CMV immediate early, HSV thymidine kinase, early and late SV40, LTRs from retrovirus, and mouse metallothionein-I. Selection of the appropriate vector and promoter is well within the level of ordinary skill in the art.

10 The host cell for recombinant production can be a higher eukaryotic cell, such as a mammalian cell, or a lower eukaryotic cell, such as a yeast cell, or the host cell can be a prokaryotic cell, such as a bacterial cell. Introduction of the construct into the host cell can be effected by calcium phosphate transfection, DEAE-Dextran mediated transfection, or electroporation (Davis, L., Dibner, M., Battey, I., Basic Methods in Molecular Biology,  
15 (1986)).

The constructs in host cells can be used in a conventional manner to produce the gene product encoded by the recombinant sequence. Alternatively, the polypeptides of the invention can be synthetically produced by conventional peptide synthesizers.

Mature proteins can be expressed in mammalian cells, yeast, bacteria, or  
20 other cells under the control of appropriate promoters. Cell-free translation systems can also be employed to produce such proteins using RNAs derived from the DNA constructs of the present invention. Appropriate cloning and expression vectors for use with prokaryotic and eukaryotic hosts, as well as other methods in molecular biology, are described in Sambrook, *et al.*, 1989, *Molecular Cloning: A Laboratory Manual*, Second Edition, Cold Spring  
25 Harbor, N.Y.; Wu *et al.*, *Methods in Gene Biotechnology* (CRC Press, New York, NY, 1997), and *Recombinant Gene Expression Protocols*, in *Methods in Molecular Biology*, Vol. 62, (Tuan, ed., Humana Press, Totowa, NJ, 1997), the disclosures of which are hereby incorporated by reference.

Transcription of the DNA encoding the polypeptides of the present invention  
30 by higher eukaryotes is increased by inserting an enhancer sequence into the vector. Enhancers are cis-acting elements of DNA, usually about from 10 to 300 bp that act on a promoter to increase its transcription. Examples include the SV40 enhancer on the late side of the replication origin bp 100 to 270, a cytomegalovirus early promoter enhancer, the polyoma enhancer on the late side of the replication origin, and adenovirus enhancers.  
35



Generally, recombinant expression vectors will include origins of replication and selectable markers permitting transformation of the host cell, *e.g.*, the ampicillin resistance gene of *E. coli* and *S. cerevisiae* TRP1 gene, and a promoter derived from a highly-expressed gene to direct transcription of a downstream structural sequence. Such promoters can be derived from operons encoding glycolytic enzymes such as 3-phosphoglycerate kinase (PGK),  $\alpha$ -factor, acid phosphatase, or heat shock proteins, among others. The heterologous structural sequence is assembled in appropriate phase with translation initiation and termination sequences. Optionally, the heterologous sequence can encode a fusion protein including an N-terminal identification peptide imparting desired characteristics, *e.g.*, stabilization or simplified purification of expressed recombinant product.

Useful expression vectors for bacterial use are constructed by inserting a structural DNA sequence encoding a desired protein together with suitable translation initiation and termination signals in operable reading phase with a functional promoter. The vector will comprise one or more phenotypic selectable markers and an origin of replication to ensure maintenance of the vector and to, if desirable, provide amplification within the host. Suitable prokaryotic hosts for transformation include *E. coli*, *Bacillus subtilis*, *Salmonella typhimurium* and various species within the genera *Pseudomonas*, *Streptomyces*, and *Staphylococcus*, although others may also be employed as a matter of choice.

As a representative but non-limiting example, useful expression vectors for bacterial use can comprise a selectable marker and bacterial origin of replication derived from commercially available plasmids comprising genetic elements of the well known cloning vector pBR322 (ATCC 37017). Such commercial vectors include, for example, pKK223-3 (Pharmacia Fine Chemicals, Uppsala, Sweden) and GEM1 (Promega Biotec, Madison, WI, USA). These pBR322 "backbone" sections are combined with an appropriate promoter and the structural sequence to be expressed.

Following transformation of a suitable host strain and growth of the host strain to an appropriate cell density, the selected promoter is induced by appropriate means (*e.g.*, temperature shift or chemical induction) and cells are cultured for an additional period.

Cells are typically harvested by centrifugation, disrupted by physical or chemical means, and the resulting crude extract retained for further purification.

Microbial cells employed in expression of proteins can be disrupted by any convenient method, including freeze-thaw cycling, sonication, a french press, mechanical disruption, or use of cell lysing agents, such methods are well known to those skilled in the art.



Various mammalian cell culture systems can also be employed to express recombinant protein. Examples of mammalian expression systems include the COS-7 lines of monkey kidney fibroblasts (described by Gluzman, 1981, *Cell*, 23:175) and other cell lines capable of expressing a compatible vector, for example, the C127, 3T3, CHO, HeLa and BHK cell lines. Mammalian expression vectors will comprise an origin of replication, a suitable promoter and enhancer, and also any necessary ribosome binding sites, polyadenylation site, splice donor and acceptor sites, transcriptional termination sequences, and 5' flanking nontranscribed sequences. DNA sequences derived from the SV40 splice, and polyadenylation sites may be used to provide the required nontranscribed genetic elements.

The proteins and polypeptides can be recovered and/or purified from recombinant cell cultures by well-known protein recovery and purification methods. Such methodology may include ammonium sulfate or ethanol precipitation, acid extraction, anion or cation exchange chromatography, phosphocellulose chromatography, hydrophobic interaction chromatography, affinity chromatography, hydroxylapatite chromatography and lectin chromatography. Protein refolding steps can be used, as necessary, in completing configuration of the mature protein. In this respect, chaperones may be used in such a refolding procedure. Finally, high performance liquid chromatography (HPLC) can be employed for final purification steps.

The polypeptides that are useful as immunogens in the present invention may be a naturally purified product (if a suitable naturally occurring mutant exists), or a product of chemical synthetic procedures, or produced by recombinant techniques from a prokaryotic or eukaryotic host (for example, by bacterial, yeast, higher plant, insect and mammalian cells in culture). Depending upon the host employed in a recombinant production procedure, the polypeptides of the present invention may be glycosylated or may be non-glycosylated. Particularly preferred immunogens are FimH adhesin protein or fragments thereof since FimH is highly conserved among many bacterial species (see Figure 3). Therefore, antibodies against FimH (or its mannose-binding fragments) should bind to FimH of other bacterial species (in addition to *E. coli*) and vaccines against *E. coli* FimH (or FimH mannose-binding fragments) should give protection against other bacterial infections in addition to *E. coli* infections (for example, against other Enterobacteriaceae infections) (see, e.g., U.S. Application Serial No. 09/615,846 and PCT application No. PCT/US00/19066, both entitled "Donor Strand Complemented Pilus-Based Vaccines" and filed July 13, 2000; U.S. Application No. 09/616,702, filed July 14, 2000, entitled "FimH Adhesin Based Vaccines" by Hultgren *et al.*; and U.S. Provisional Application No. 60/216,750, filed July 7,



2000, entitled "FimH Adhesin Proteins" by Langermann *et al.*)

Procedures for the isolation of a periplasmic chaperone protein complexed with an adhesin protein are known in the art, as an example see Jones *et al.*, (1993, *Proc. Natl. Acad. Sci. USA* 90:8397-8401). Further, the individually expressed adhesin proteins may be isolated by recombinant expression/isolation methods that are well-known in the art. Typical examples for such isolation may utilize an antibody to the protein or to a His tag or cleavable leader or tail that is expressing as part of the protein structure.

The FimCH polypeptides useful in forming the vaccine compositions of the present invention may conveniently be cloned using various cloning systems. The FimCH complex described therein is composed of a 52 kDa complex composed of two proteins: FimC (22.8 kDa) and FimH (29.1 kDa) in a 1:1 equimolar ratio. The FimCH complex is expressed from a pUC-based vector (pGCA139-1-1) with two separate lac-inducible promoters driving expression of the FimC and FimH genes, respectively. The FimC and the FimH genes in the pGCA139-1-1 vector were derived from uropathogenic *E. coli* isolate J96 and have the nucleotide sequences of Figure 1.

The FimCH complex is produced in the periplasm of *E. coli* strain BL21 and is purified from periplasmic extracts by standard chromatographic methods. The FimCH protein has been formulated in a number of different buffers compatible with its solubility profile including 20 mM HEPES (pH 7.0), PBS (pH 7.0) and sodium citrate (pH 6.0) in 0.2 M NaCl. This sodium citrate/sodium chloride formulation enhances the stability of the FimCH complex and is also compatible with commonly used diluents.

Plasmid pCGA139-1-1 was constructed as a means of producing relatively large amounts of *E. coli* chaperone-adhesin complex, wild type FimCH. For use in the vaccine compositions disclosed herein, the wild type FimH is replaced with a mutant FimH.

The plasmid vector, pCGA139-1-1, contains the following genetic elements: (1) an *E. coli* FimC chaperone gene followed by (2) the FimH adhesin gene, both from *E. coli* strain J96 (a urinary tract infection (UTI) isolate) each preceded by its respective native signal sequence (*nss*); (3) a kanamycin resistance (*kan<sup>r</sup>* or *k<sup>r</sup>*) marker; (4) *lacI<sup>q</sup>* which codes for a repressor protein that binds the *lac* promoter unless it is induced; (5) an inactivated beta-lactamase (*bla*) gene; (6) pUC origin of replication (*ori*); and (7) two *lac* promoters, one preceding the FimC signal and the other preceding that of FimH.



### 5.6.1 FUSION PROTEINS

In certain embodiments, the invention provides a polypeptide which is constructed as a fusion protein (*e.g.*, covalently bonded to a different protein). The invention provides nucleic acids encoding such fusion proteins. In certain other  
5       embodiments of this invention, the nucleic acid encoding a fusion protein of the invention is operably linked to an appropriate promoter.

Fusion proteins in which a mutant FimH protein, preferably an adhesion or FimH, or a fragment of such a protein is fused to a heterologous protein are within the scope of this invention. In addition, fusion proteins can be made with antibodies of the invention  
10       or fragments thereof. Such proteins and peptides can be designed, for example, on the basis of the nucleotide sequences disclosed herein and/or on the basis of the amino acid sequences disclosed herein. Fusion proteins include, but are not limited to fusions to any amino acid sequence that allows the fusion protein to be anchored to the cell membrane; or fusions of the peptide to an enzyme, fluorescent protein, luminescent protein, or a flag epitope protein  
15       or peptide which provides a marker function.

In a specific embodiment, a polypeptide of the invention (or a nucleic acid encoding the polypeptide of the invention) is constructed as a chimeric or fusion protein. The polypeptide of the invention is joined at its amino- or carboxy-terminus via a peptide bond to an amino acid sequence of a different protein. In specific embodiments, the amino  
20       acid sequence of the different protein is at least 6, 10, 20 or 30 continuous amino acids of the different proteins or a portion of the heterologous protein that is functionally active. In specific embodiments, the amino acid sequence of the different protein is at least 50, 75, 100, or 150 continuous amino acids of the different proteins or a portion of the different protein that is functionally active. In one embodiment, such a chimeric protein is produced  
25       by recombinant expression of a nucleic acid encoding a polypeptide of the invention joined in-frame to a coding sequence for a different protein (*e.g.*, such as a heparin binding domain). Such a chimeric product can be made by ligating the appropriate nucleic acid sequences encoding the desired amino acid sequences to each other by methods known in the art, in the proper coding frame, and expressing the chimeric product into the expression  
30       vehicle of choice by methods commonly known in the art.

Chimeric nucleic acids comprising portions of a nucleic acid encoding a polypeptide of the invention fused to any heterologous protein-encoding sequences may be constructed. In a specific embodiment, the fusion protein comprises an affinity tag such as a  
35       hexahistidine tag, or other affinity tag that may be used in purification, isolation,



identification, or assay of expression. In another specific embodiment, the fusion protein comprises a protease cleavage site such as a metal protease or serine cleavage site.

Construction of fusion proteins for expression in bacteria or eukaryotic systems are well known in the art and such methods are within the scope of the invention.

5 Any fusion protein may be readily purified by utilizing an antibody specific for the fusion protein being expressed. For example, a system described by Janknecht *et al.* (1991, *Proc. Natl. Acad. Sci. USA* 88:8972-8976) allows for the ready purification of non-denatured fusion proteins expressed in human cell lines. In this system, the nucleic acid of interest is subcloned into a vaccinia recombination plasmid such that the open reading frame is translationally fused to an amino-terminal tag consisting of six histidine residues.  
10 Extracts from cells infected with recombinant vaccinia virus are loaded onto  $\text{Ni}^{2+}$ -nitriloacetic acid-agarose columns and histidine-tagged proteins are selectively eluted with imidazole-containing buffers.

## 15 **5.7 ANTIBODIES GENERATED BY THE VACCINES OF THE INVENTION**

Antibodies generated against mutant proteins of the invention by immunization with the vaccines formulations of the present invention also have potential uses in diagnostic assays, passive immunotherapy, and generation of antiidiotypic antibodies.

20 Techniques described for the production of single chain antibodies (U.S. Patent 4,946,778) can be adapted to produce single chain antibodies to immunogenic mutant polypeptide products of this invention. Also, transgenic mice may be used to express humanized antibodies to immunogenic mutant polypeptide products of this invention.

The vaccine formulations of the present invention can also be used to  
25 produce antibodies for use in passive immunotherapy, in which short-term protection of a host is achieved by the administration of pre-formed antibody directed against a heterologous organism.

More particularly, an isolated mutant polypeptide of the invention, or a fragment thereof, can be used as an immunogen to generate antibodies using standard  
30 techniques for polyclonal and monoclonal antibody preparation. The full-length mutant polypeptide or protein can be used or, alternatively, the invention provides antigenic peptide fragments for use as immunogens. The antigenic peptide of a mutant protein of the invention comprises at least 8 (preferably 10, 15, 20, or 30) amino acid residues, and encompasses an epitope of the mutant protein such that an antibody raised against the  
35 peptide forms a specific immune complex with the protein.



Preferred epitopes encompassed by an antigenic mutant protein are regions that are located on the surface of the protein, *e.g.*, hydrophilic regions. In certain embodiments, the nucleic acid molecules of the invention are present as part of nucleic acid molecules comprising nucleotide sequences that contain or encode heterologous (*e.g.*,  
5 vector, expression vector, or fusion protein) sequences. These nucleotides can then be used to express proteins which can be used as immunogens to generate an immune response, or more particularly, to generate polyclonal or monoclonal antibodies specific to the expressed protein.

10 An immunogen typically is used to prepare antibodies by immunizing a suitable subject, (*e.g.*, rabbit, goat, mouse or other mammal). An appropriate immunogenic preparation can contain, for example, recombinantly expressed or chemically synthesized mutant polypeptide. The preparation can further include an adjuvant, such as Freund's complete or incomplete adjuvant, or similar immunostimulatory agent.

15 Accordingly, another aspect of the invention pertains to antibodies directed against a polypeptide of the invention. The term "antibody" as used herein refers to immunoglobulin molecules and immunologically active portions of immunoglobulin molecules, *i.e.*, molecules that contain an antigen binding site which specifically binds an antigen, such as a polypeptide of the invention, *e.g.*, an epitope of a polypeptide of the invention. A molecule which specifically binds to a given polypeptide of the invention is a  
20 molecule which binds the polypeptide, but does not substantially bind other molecules in a sample, *e.g.*, a biological sample, which naturally contains the polypeptide. Examples of immunologically active portions of immunoglobulin molecules include F(ab) and F(ab')<sub>2</sub> fragments which can be generated by treating the antibody with an enzyme such as pepsin. The invention provides polyclonal and monoclonal antibodies. The term "monoclonal  
25 antibody" or "monoclonal antibody composition", as used herein, refers to a population of antibody molecules that contain only one species of an antigen binding site capable of immunoreacting with a particular epitope.

30 Polyclonal antibodies can be prepared by immunizing a suitable subject with a mutant polypeptide of the invention as an immunogen. Preferred polyclonal antibody compositions are ones that have been selected for antibodies directed against a polypeptide or polypeptides of the invention. Particularly preferred polyclonal antibody preparations are ones that contain only antibodies directed against a polypeptide or polypeptides of the invention. Particularly preferred immunogen compositions are those that contain no other human proteins such as, for example, immunogen compositions made using a non-human  
35 host cell for recombinant expression of a polypeptide of the invention. In such a manner, the



only human epitope or epitopes recognized by the resulting antibody compositions raised against this immunogen will be present as part of a polypeptide or polypeptides of the invention.

5 The antibody titer in the immunized subject can be monitored over time by standard techniques, such as with an enzyme linked immunosorbent assay (ELISA) using immobilized polypeptide. If desired, the antibody molecules can be isolated from the mammal (*e.g.*, from the blood) and further purified by well-known techniques, such as protein A chromatography to obtain the IgG fraction. Alternatively, antibodies specific for a protein or polypeptide of the invention can be selected for (*e.g.*, partially purified) or  
10 purified by, *e.g.*, affinity chromatography. For example, a recombinantly expressed and purified (or partially purified) protein of the invention is produced as described herein, and covalently or non-covalently coupled to a solid support such as, for example, a chromatography column. The column can then be used to affinity purify antibodies specific for the proteins of the invention from a sample containing antibodies directed against a large  
15 number of different epitopes, thereby generating a substantially purified antibody composition, *i.e.*, one that is substantially free of contaminating antibodies. By a substantially purified antibody composition is meant, in this context, that the antibody sample contains at most only 30% (by dry weight) of contaminating antibodies directed against epitopes other than those on the desired protein or polypeptide of the invention, and  
20 preferably at most 20%, yet more preferably at most 10%, and most preferably at most 5% (by dry weight) of the sample is contaminating antibodies. A purified antibody composition means that at least 99% of the antibodies in the composition are directed against the desired protein or polypeptide of the invention.

25 At an appropriate time after immunization, *e.g.*, when the specific antibody titers are highest, antibody-producing cells can be obtained from the subject and used to prepare monoclonal antibodies by standard techniques, such as the hybridoma technique (originally described by Kohler and Milstein, 1975, *Nature* 256:495-497), the human B cell hybridoma technique (Kozbor *et al.*, 1983, *Immunol. Today* 4:72), the EBV-hybridoma technique (Cole *et al.*, 1985, *Monoclonal Antibodies and Cancer Therapy*, Alan R. Liss, Inc., pp. 77-96) or trioma techniques. The technology for producing hybridomas is well  
30 known (*see generally Current Protocols in Immunology* (1994) Coligan *et al.* (eds.) John Wiley & Sons, Inc., New York, NY). Hybridoma cells producing a monoclonal antibody of the invention are detected by screening the hybridoma culture supernatants for antibodies that bind the polypeptide of interest, *e.g.*, using a standard ELISA assay.

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Alternative to preparing monoclonal antibody-secreting hybridomas, a monoclonal antibody directed against a polypeptide of the invention can be identified and isolated by screening a recombinant combinatorial immunoglobulin library (e.g., an antibody phage display library) with the polypeptide of interest. Kits for generating and screening phage display libraries are commercially available (e.g., the Pharmacia *Recombinant Phage Antibody System*, Catalog No. 27-9400-01; and the Stratagene *SurfZAP Phage Display Kit*, Catalog No. 240612). Additionally, examples of methods and reagents particularly amenable for use in generating and screening antibody display library can be found in, for example, U.S. Patent No. 5,223,409; PCT Publication No. WO 92/18619; PCT Publication No. WO 91/17271; PCT Publication No. WO 92/20791; PCT Publication No. WO 92/15679; PCT Publication No. WO 93/01288; PCT Publication No. WO 92/01047; PCT Publication No. WO 92/09690; PCT Publication No. WO 90/02809; Fuchs *et al.*, 1991, *BioTechnology* 9:1370-1372; Hay *et al.*, 1992, *Hum. Antibod. Hybridomas* 3:81-85; Huse *et al.*, 1989, *Science* 246:1275-1281; Griffiths *et al.*, 1993, *EMBO J.* 12:725-734.

Additionally, recombinant antibodies, such as chimeric and humanized monoclonal antibodies, comprising both human and non-human portions, which can be made using standard recombinant DNA techniques, are within the scope of the invention. A chimeric antibody is a molecule in which different portions are derived from different animal species, such as those having a variable region derived from a murine MAB and a human immunoglobulin constant region. (See, e.g., Cabilly *et al.*, U.S. Patent No. 4,816,567; and Boss *et al.*, U.S. Patent No. 4,816,397, which are incorporated herein by reference in their entirety.) Humanized antibodies are antibody molecules from non-human species having one or more complementarily determining regions (CDRs) from the non-human species and a framework region from a human immunoglobulin molecule. (See, e.g., Queen, U.S. Patent No. 5,585,089, which is incorporated herein by reference in its entirety.) Such chimeric and humanized monoclonal antibodies can be produced by recombinant DNA techniques known in the art, for example using methods described in PCT Publication No. WO 87/02671; European Patent Application 184,187; European Patent Application 171,496; European Patent Application 173,494; PCT Publication No. WO 86/01533; U.S. Patent No. 4,816,567; European Patent Application 125,023; Better *et al.*, 1988, *Science* 240:1041-1043; Liu *et al.*, 1987, *Proc. Natl. Acad. Sci. USA* 84:3439-3443; Liu *et al.*, 1987, *J. Immunol.* 139:3521-3526; Sun *et al.*, 1987, *Proc. Natl. Acad. Sci. USA* 84:214-218; Nishimura *et al.*, 1987, *Canc. Res.* 47:999-1005; Wood *et al.*, 1985, *Nature* 314:446-449; and Shaw *et al.*, 1988, *J. Natl. Cancer Inst.* 80:1553-1559; Morrison, 1985, *Science* 229:1202-1207; Oi *et al.*, 1986, *BioTechniques* 4:214; U.S. Patent 5,225,539; Jones *et al.*,



1986, *Nature* 321:552-525; Verhoeyan *et al.*, 1988, *Science* 239:1534; and Beidler *et al.*, 1988, *J. Immunol.* 141:4053-4060.

Completely human antibodies are particularly desirable for therapeutic treatment of human patients. Such antibodies can be produced, for example, using transgenic mice which are incapable of expressing endogenous immunoglobulin heavy and light chains genes, but which can express human heavy and light chain genes. The transgenic mice are immunized in the normal fashion with a selected antigen, *e.g.*, all or a portion of a polypeptide of the invention. Monoclonal antibodies directed against the antigen can be obtained using conventional hybridoma technology. The human immunoglobulin transgenes harbored by the transgenic mice rearrange during B cell differentiation, and subsequently undergo class switching and somatic mutation. Thus, using such a technique, it is possible to produce therapeutically useful IgG, IgA and IgE antibodies. For an overview of this technology for producing human antibodies, see Lonberg and Huszar (1995, *Int. Rev. Immunol.* 13:65-93). For a detailed discussion of this technology for producing human antibodies and human monoclonal antibodies and protocols for producing such antibodies, *see, e.g.*, U.S. Patent 5,625,126; U.S. Patent 5,633,425; U.S. Patent 5,569,825; U.S. Patent 5,661,016; and U.S. Patent 5,545,806. In addition, companies such as Abgenix, Inc. (Freemont, CA), can be engaged to provide human antibodies directed against a selected antigen using technology similar to that described above.

Completely human antibodies which recognize a selected epitope can be generated using a technique referred to as "guided selection." In this approach a selected non-human monoclonal antibody, *e.g.*, a mouse antibody, is used to guide the selection of a completely human antibody recognizing the same epitope. (Jespers *et al.*, 1994, *BioTechnology* 12:899-903).

An antibody directed against a polypeptide of the invention can be used to detect the protein (*e.g.*, in a cellular lysate or cell supernatant) in order to evaluate the abundance and pattern of expression of the polypeptide. The antibodies can also be used diagnostically to monitor protein levels in tissue as part of a clinical testing procedure, *e.g.*, to, for example, determine the efficacy of a given treatment regimen. Detection can be facilitated by coupling the antibody to a detectable substance. Examples of detectable substances include various enzymes, prosthetic groups, fluorescent materials, luminescent materials, bioluminescent materials, and radioactive materials. Examples of suitable enzymes include horseradish peroxidase, alkaline phosphatase, beta-galactosidase, or acetylcholinesterase; examples of suitable prosthetic group complexes include streptavidin/biotin and avidin/biotin; examples of suitable fluorescent materials include



umbelliferone, fluorescein, fluorescein isothiocyanate, rhodamine, dichlorotriazinylamine fluorescein, dansyl chloride or phycoerythrin; an example of a luminescent material includes luminol; examples of bioluminescent materials include luciferase, luciferin, and aequorin, and examples of suitable radioactive material include  $^{125}\text{I}$ ,  $^{131}\text{I}$ ,  $^{35}\text{S}$  or  $^3\text{H}$ .

5 In addition, gene sequences and gene products of the invention, including peptide fragments, as well as specific antibodies thereto, can be used for construction of fusion proteins to facilitate recovery, detection, or localization of another protein of interest.

Further, an antibody (or fragment thereof) may be conjugated to a therapeutic moiety such as a cytotoxin, a therapeutic agent or a radioactive metal ion. A cytotoxin or  
10 cytotoxic agent includes any agent that is detrimental to cells, and in particular, prokaryotic cells.

The conjugates of the invention can be used for modifying a given biological response, the drug moiety is not to be construed as limited to classical chemical therapeutic agents. For example, the drug moiety may be a protein or polypeptide possessing a desired  
15 biological activity. Such proteins may include, for example, a toxin such as abrin, ricin A, pseudomonas exotoxin, or diphtheria toxin; a protein such as tumor necrosis factor,  $\alpha$ -interferon,  $\beta$ -interferon, nerve growth factor, platelet derived growth factor, tissue plasminogen activator, a thrombotic agent or an anti-angiogenic agent, *e.g.*, angiostatin or endostatin; or, biological response modifiers such as, for example, lymphokines, interleukin-  
20 1 ("IL-1"), interleukin-2 ("IL-2"), interleukin-6 ("IL-6"), granulocyte macrophage colony stimulating factor ("GM-CSF"), granulocyte colony stimulating factor ("G-CSF"), interleukin-10 ("IL-10"), interleukin-12 ("IL-12"), interferon- $\gamma$  ("IFN- $\gamma$ "), interferon- $\alpha$  ("IFN- $\alpha$ "), or other immune factors or growth factors.

Techniques for conjugating such therapeutic moiety to antibodies are well  
25 known, see, *e.g.*, Arnon *et al.*, "Monoclonal Antibodies For Immunotargeting Of Drugs In Cancer Therapy", in Monoclonal Antibodies And Cancer Therapy, Reisfeld *et al.* (eds.), pp. 243-56 (Alan R. Liss, Inc. 1985); Hellstrom *et al.*, "Antibodies For Drug Delivery", in Controlled Drug Delivery (2nd Ed.), Robinson *et al.* (eds.), pp. 623-53 (Marcel Dekker, Inc. 1987); Thorpe, "Antibody Carriers Of Cytotoxic Agents In Cancer Therapy: A Review", in  
30 Monoclonal Antibodies '84: Biological And Clinical Applications, Pinchera *et al.* (eds.), pp. 475-506 (1985); "Analysis, Results, And Future Prospective Of The Therapeutic Use Of Radiolabeled Antibody In Cancer Therapy", in Monoclonal Antibodies For Cancer Detection And Therapy, Baldwin *et al.* (eds.), pp. 303-16 (Academic Press 1985), and Thorpe *et al.*, 1982, *Immunol. Rev.*, 62:119-58.



An antibody with or without a therapeutic moiety conjugated to it can be used as a therapeutic that is passively administered alone or in combination with chemotherapeutic agents.

5 Alternatively, an antibody of the invention can be conjugated to a second antibody to form an "antibody heteroconjugate" as described by Segal in U.S. Patent No. 4,676,980 or alternatively, the antibodies can be conjugated to form an "antibody heteropolymer" as described in Taylor *et al.*, in U.S. Patent Nos. 5,470,570 and 5,487,890.

10 An antibody with or without a therapeutic moiety conjugated to it can be used as a therapeutic that is administered alone or in combination with cytotoxic factor(s) and/or cytokine(s).

In yet a further aspect, the invention provides substantially purified antibodies or fragments thereof, including human or non-human antibodies or fragments thereof, which antibodies or fragments specifically bind to a polypeptide of the invention. In various embodiments, the substantially purified antibodies of the invention, or fragments thereof,  
15 can be human, non-human, chimeric and/or humanized antibodies.

In another aspect, the invention provides non-human antibodies or fragments thereof. Such non-human antibodies can be goat, mouse, sheep, horse, chicken, rabbit, or rat antibodies. Alternatively, the non-human antibodies of the invention can be chimeric and/or humanized antibodies. In addition, the non-human antibodies of the invention can be  
20 polyclonal antibodies or monoclonal antibodies.

In still a further aspect, the invention provides monoclonal antibodies or fragments thereof. The monoclonal antibodies can be human, humanized, chimeric and/or non-human antibodies.

25 Any of the antibodies of the invention can be conjugated to a therapeutic moiety or to a detectable substance. Non-limiting examples of detectable substances that can be conjugated to the antibodies of the invention are an enzyme, a prosthetic group, a fluorescent material, a luminescent material, a bioluminescent material, and a radioactive material.

30 The invention also provides a kit containing an antibody of the invention conjugated to a detectable substance, and instructions for use. Still another aspect of the invention is a pharmaceutical composition comprising an antibody of the invention and a pharmaceutically acceptable carrier. In preferred embodiments, the pharmaceutical composition contains an antibody of the invention, a therapeutic moiety, and a  
35 pharmaceutically acceptable carrier.



After immunization, a sample is collected from the mammal that contains an antibody that specifically recognizes the immunogen. Preferably, the polypeptide is recombinantly produced using a non-human host cell. Optionally, the antibodies can be further purified from the sample using techniques well known to those of skill in the art.

5 The method can further comprise producing a monoclonal antibody-producing cell from the cells of the mammal. Optionally, antibodies are collected from the antibody-producing cell.

### 5.8 RECOMBINANT METHODS OF PRODUCING ANTIBODIES

10 The antibodies of the invention or fragments thereof can be produced by any method known in the art for the synthesis of antibodies, in particular, by chemical synthesis or preferably, by recombinant expression techniques.

The nucleotide sequence encoding an antibody of the invention can be obtained from sequencing hybridoma clone DNA. If a clone containing a nucleic acid encoding a particular antibody or an epitope-binding fragment thereof is not available, but  
15 the sequence of the antibody molecule or epitope-binding fragment thereof is known, a nucleic acid encoding the immunoglobulin may be chemically synthesized or obtained from a suitable source (*e.g.*, an antibody cDNA library, or a cDNA library generated from, or nucleic acid, preferably poly A<sup>+</sup> RNA, isolated from any tissue or cells expressing the antibody, such as hybridoma cells selected to express an antibody) by PCR amplification  
20 using synthetic primers hybridizable to the 3' and 5' ends of the sequence or by cloning using an oligonucleotide probe specific for the particular gene sequence to identify, *e.g.*, a cDNA clone from a cDNA library that encodes the antibody. Amplified nucleic acids generated by PCR may then be cloned into replicable cloning vectors using any method well known in the art.

25 Once the nucleotide sequence of the antibody is determined, the nucleotide sequence of the antibody may be manipulated using methods well known in the art for the manipulation of nucleotide sequences, *e.g.*, recombinant DNA techniques, site directed mutagenesis, PCR, etc. (see, for example, the techniques described in Sambrook *et al.*, 1990, *Molecular Cloning, A Laboratory Manual*, 2d Ed., Cold Spring Harbor Laboratory, Cold  
30 Spring Harbor, NY; and Ausubel *et al.*, eds., 1998, *Current Protocols in Molecular Biology*, John Wiley & Sons, NY, which are both incorporated by reference herein in their entireties), to generate antibodies having a different amino acid sequence by, for example, introducing amino acid substitutions, deletions, and/or insertions into the epitope-binding domain regions of the antibodies and preferably, into the hinge-Fc regions of the antibodies which  
35 are involved in the interaction with the FcRn. In a preferred embodiment, antibodies having



one or more modifications in amino acid residues 251-256, amino acid residues 285-290, amino acid residues 308-314, amino acid residues 382-386, and/or amino acid residues 428-436 are generated.

5 Recombinant expression of an antibody requires construction of an expression vector containing a nucleotide sequence that encodes the antibody. Once a nucleotide sequence encoding an antibody molecule or a heavy or light chain of an antibody, or portion thereof (preferably, but not necessarily, containing the heavy or light chain variable region) has been obtained, the vector for the production of the antibody molecule may be produced by recombinant DNA technology using techniques well known in the art. 10 Thus, methods for preparing a protein by expressing a polynucleotide containing an antibody encoding nucleotide sequence are described herein. Methods which are well known to those skilled in the art can be used to construct expression vectors containing antibody coding sequences and appropriate transcriptional and translational control signals. These methods include, for example, *in vitro* recombinant DNA techniques, synthetic techniques, and *in vivo* genetic recombination. The invention, thus, provides replicable vectors comprising a 15 nucleotide sequence encoding the constant region of the antibody molecule with one or more modifications in the amino acid residues involved in the interaction with the FcRn (see, e.g., PCT Publication WO 86/05807; PCT Publication WO 89/01036; U.S. Patent No. 5,122,464; Provisional Patent Application 60/254,880, filed December 12, 2000 by Johnson et al.; and 20 Provisional Patent Application 60/289,760, filed May 9, 2001 by Johnson et al.). The nucleotide sequence encoding the heavy-chain variable region, light-chain variable region, both the heavy-chain and light-chain variable regions, an epitope-binding fragment of the heavy- and/or light-chain variable region, or one or more complementarity determining regions (CDRs) of an antibody may be cloned into such a vector for expression.

25 The expression vector is transferred to a host cell by conventional techniques and the transfected cells are then cultured by conventional techniques to produce an antibody having an increased affinity for the FcRn and an increased *in vivo* half-life. Thus, the invention includes host cells containing a polynucleotide encoding an antibody, an hinge-Fc region or fragments thereof (*i.e.*, constant regions) having one or more modifications in 30 amino acid residues 251-256, amino acid residues 285-290, amino acid residues 308-314, amino acid residues 382-386, and/or amino acid residues 428-436, operably linked to a heterologous promoter.

A variety of host-expression vector systems may be utilized to express the antibody molecules of the invention. Such host-expression systems represent vehicles by 35 which the coding sequences of interest may be produced and subsequently purified, but also



represent cells which may, when transformed or transfected with the appropriate nucleotide coding sequences, express an antibody molecule of the invention *in situ*. These include but are not limited to microorganisms such as bacteria (*e.g.*, *E. coli* and *B. subtilis*) transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors  
5 containing antibody coding sequences; yeast (*e.g.*, *Saccharomyces* and *Pichia*) transformed with recombinant yeast expression vectors containing antibody coding sequences; insect cell systems infected with recombinant virus expression vectors (*e.g.*, baculovirus) containing antibody coding sequences; plant cell systems infected with recombinant virus expression  
10 vectors (*e.g.*, cauliflower mosaic virus, CaMV; and tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (*e.g.*, Ti plasmid) containing antibody coding sequences; and mammalian cell systems (*e.g.*, COS, CHO, BHK, 293, 3T3, and NS0 cells) harboring recombinant expression constructs containing promoters derived from the genome of mammalian cells (*e.g.*, metallothionein promoter) or from mammalian  
15 viruses (*e.g.*, the adenovirus late promoter; the vaccinia virus 7.5K promoter). Preferably, bacterial cells such as *Escherichia coli*, and more preferably, eukaryotic cells, especially for the expression of whole recombinant antibody molecule, are used for the expression of a recombinant antibody molecule. For example, mammalian cells such as Chinese hamster ovary cells (CHO), in conjunction with a vector such as the major intermediate early gene promoter element from human cytomegalovirus is an effective expression system for  
20 antibodies (Foecking *et al.*, *Gene*, 45:101, 1986, and Cockett *et al.*, *BioTechnology*, 8:2, 1990).

In bacterial systems, a number of expression vectors may be advantageously selected depending upon the use intended for the antibody molecule being expressed. For example, when a large quantity of such a protein is to be produced, for the generation of  
25 pharmaceutical compositions of an antibody molecule, vectors which direct the expression of high levels of fusion protein products that are readily purified may be desirable. Such vectors include, but are not limited to, the *E. coli* expression vector pUR278 (Ruther *et al.*, 1983, *EMBO* 12:1791), in which the antibody coding sequence may be ligated individually into the vector in frame with the lacZ coding region so that a fusion protein is produced; and  
30 pIN vectors (Inouye & Inouye, 1985, *Nucleic Acids Res.*, 13:3101-3109; Van Heeke & Schuster, 1989, *J. Biol. Chem.* 24:5503-5509).

In an insect system, Autographa californica nuclear polyhedrosis virus (AcNPV) is used as a vector to express foreign genes. The virus grows in *Spodoptera frugiperda* cells. The antibody coding sequence may be cloned individually into non-  
35 essential regions (for example the polyhedrin gene) of the virus and placed under control of



an AcNPV promoter (for example the polyhedrin promoter).

In mammalian host cells, a number of viral-based expression systems may be utilized to express an antibody molecule of the invention. In cases where an adenovirus is used as an expression vector, the antibody coding sequence of interest may be ligated to an  
5 adenovirus transcription/translation control complex, *e.g.*, the late promoter and tripartite leader sequence. This chimeric gene may then be inserted in the adenovirus genome by *in vitro* or *in vivo* recombination. Insertion in a non-essential region of the viral genome (*e.g.*, region E1 or E3) will result in a recombinant virus that is viable and capable of expressing the antibody molecule in infected hosts (*e.g.*, see Logan & Shenk, *Proc. Natl. Acad. Sci.*  
10 *USA*, 81:355-359, 1984). Specific initiation signals may also be required for efficient translation of inserted antibody coding sequences. These signals include the ATG initiation codon and adjacent sequences. Furthermore, the initiation codon must be in phase with the reading frame of the desired coding sequence to ensure translation of the entire insert. These  
15 exogenous translational control signals and initiation codons can be of a variety of origins, both natural and synthetic. The efficiency of expression may be enhanced by the inclusion of appropriate transcription enhancer elements, transcription terminators, etc. (see, *e.g.*, Bitter *et al.*, *Methods in Enzymol.*, 153:516-544, 1987).

In addition, a host cell strain may be chosen which modulates the expression of the antibody sequences, or modifies and processes the antibody in the specific fashion  
20 desired. Such modifications (*e.g.*, glycosylation) and processing (*e.g.*, cleavage) of protein products may be important for the function of the antibody. Different host cells have characteristic and specific mechanisms for the post-translational processing and modification of proteins and gene products. Appropriate cell lines or host systems can be chosen to ensure the correct modification and processing of the antibody expressed. To this  
25 end, eukaryotic host cells which possess the cellular machinery for proper processing of the primary transcript, glycosylation, and phosphorylation of the gene product may be used. Such mammalian host cells include but are not limited to CHO, VERO, BHK, HeLa, COS, MDCK, 293, 3T3, W138, NS0 and in particular, breast cancer cell lines such as, for example, BT483, Hs578T, HTB2, BT20 and T47D, and normal mammary gland cell line  
30 such as, for example, CRL7030 and HsS78Bst.

For long-term, high-yield production of recombinant antibodies, stable expression is preferred. For example, cell lines which stably express the antibody molecule may be engineered. Rather than using expression vectors which contain viral origins of replication, host cells can be transformed with DNA controlled by appropriate expression  
35 control elements (*e.g.*, promoter, enhancer, sequences, transcription terminators,



polyadenylation sites, etc.), and a selectable marker. Following the introduction of the foreign DNA, engineered cells may be allowed to grow for 1-2 days in an enriched media, and then are switched to a selective media. The selectable marker in the recombinant plasmid confers resistance to the selection and allows cells to stably integrate the plasmid into their chromosomes and grow to form foci which in turn can be cloned and expanded into cell lines. This method may advantageously be used to engineer cell lines which express the antibody molecule. Such engineered cell lines may be particularly useful in screening and evaluation of compositions that interact directly or indirectly with the antibody molecule.

A number of selection systems may be used, including but not limited to, the herpes simplex virus thymidine kinase (Wigler *et al.*, *Cell*, 11:223, 1977), hypoxanthine guanine phosphoribosyltransferase (Szybalska & Szybalski, *Proc. Natl. Acad. Sci. USA*, 48:202, 1992), and adenine phosphoribosyltransferase (Lowy *et al.*, *Cell*, 22:8-17, 1980) genes can be employed in tk-, hgp<sup>r</sup>t- or ap<sup>r</sup>t- cells, respectively. Also, antimetabolite resistance can be used as the basis of selection for the following genes: *dhfr*, which confers resistance to methotrexate (Wigler *et al.*, *Proc. Natl. Acad. Sci. USA*, 77:357, 1980 and O'Hare *et al.*, *Proc. Natl. Acad. Sci. USA*, 78:1527, 1981); *gpt*, which confers resistance to mycophenolic acid (Mulligan & Berg, *Proc. Natl. Acad. Sci. USA*, 78:2072, 1981); neo, which confers resistance to the aminoglycoside G-418 (Wu and Wu, *Biotherapy*, 3:87-95, 1991; Tolstoshev, *Ann. Rev. Pharmacol. Toxicol.*, 32:573-596, 1993; Mulligan, *Science*, 260:926-932, 1993; and Morgan and Anderson, *Ann. Rev. Biochem.*, 62: 191-217, 1993; and May, *TIB TECH*, 11(5):155-215, 1993); and *hygro*, which confers resistance to hygromycin (Santerre *et al.*, *Gene*, 30:147, 1984). Methods commonly known in the art of recombinant DNA technology may be routinely applied to select the desired recombinant clone, and such methods are described, for example, in Ausubel *et al.* (eds.), 1993, *Current Protocols in Molecular Biology*, John Wiley & Sons, NY; Kriegler, 1990, *Gene Transfer and Expression, A Laboratory Manual*, Stockton Press, NY; in Chapters 12 and 13, Dracopoli *et al.* (eds), 1994, *Current Protocols in Human Genetics*, John Wiley & Sons, NY; and Colberre-Garapin *et al.*, *J. Mol. Biol.*, 150:1, 1981, which are incorporated by reference herein in their entirety.

The expression levels of an antibody molecule can be increased by vector amplification (for a review, see Bebbington and Hentschel, 1987, *The use of vectors based on gene amplification for the expression of cloned genes in mammalian cells in DNA cloning*, Vol.3. Academic Press, New York). When a marker in the vector system expressing antibody is amplifiable, increase in the level of inhibitor present in culture of host



cell will increase the number of copies of the marker gene. Since the amplified region is associated with the antibody gene, production of the antibody will also increase (Crouse *et al.*, 1983, *Mol. Cell. Biol.*, 3:257).

5 The host cell may be co-transfected with two expression vectors of the invention, the first vector encoding a heavy chain derived polypeptide and the second vector encoding a light chain derived polypeptide. The two vectors may contain identical selectable markers which enable equal expression of heavy and light chain polypeptides. Alternatively, a single vector may be used which encodes, and is capable of expressing, both heavy and light chain polypeptides. In such situations, the light chain should be placed  
10 before the heavy chain to avoid an excess of toxic free heavy chain (Proudfoot, *Nature*, 322:52, 1986; and Kohler, *Proc. Natl. Acad. Sci. USA*, 77:2 197, 1980). The coding sequences for the heavy and light chains may comprise cDNA or genomic DNA.

Once an antibody molecule of the invention has been produced by recombinant expression, it may be purified by any method known in the art for purification  
15 of an immunoglobulin molecule, for example, by chromatography (*e.g.*, ion exchange, affinity, particularly by affinity for the specific antigen after Protein A purification, and sizing column chromatography), centrifugation, differential solubility, or by any other standard techniques for the purification of proteins. Further, the antibodies of the present invention or fragments thereof may be fused to heterologous polypeptide sequences  
20 described herein or otherwise known in the art to facilitate purification.

### 5.8.1 ANTIBODY CONJUGATES

The present invention encompasses antibodies recombinantly fused or chemically conjugated (including both covalently and non-covalently conjugations) to  
25 heterologous polypeptides (*i.e.*, an unrelated polypeptide; or portion thereof, preferably at least 10, at least 20, at least 30, at least 40, at least 50, at least 60, at least 70, at least 80, at least 90 or at least 100 amino acids of the polypeptide) to generate fusion proteins. The fusion does not necessarily need to be direct, but may occur through linker sequences. Antibodies fused or conjugated to heterologous polypeptides may also be used in *in vitro*  
30 immunoassays and purification methods using methods known in the art. See *e.g.*, PCT publication Number WO 93/2 1232; EP 439,095; Naramura *et al.*, 1994, *Immunol. Lett.*, 39:91-99; U.S. Patent 5,474,981; Gillies *et al.*, 1992, *Proc. Natl. Acad. Sci. USA*, 89:1428-1432; and Fell *et al.*, 1991, *J. Immunol.*, 146:2446-2452, which are incorporated herein by reference in their entireties.

35 Antibodies can be fused to marker sequences, such as a peptide to facilitate



purification. In preferred embodiments, the marker amino acid sequence is a hexa-histidine peptide, such as the tag provided in a pQE vector (QIAGEN, Inc.), among others, many of which are commercially available. As described in Gentz *et al.*, 1989, *Proc. Natl. Acad. Sci. USA* 86:821-824, for instance, hexa-histidine provides for convenient purification of the fusion protein. Other peptide tags useful for purification include, but are not limited to, the hemagglutinin "HA" tag, which corresponds to an epitope derived from the influenza hemagglutinin protein (Wilson *et al.*, 1984, *Cell*, 37:767) and the "flag" tag (Knappik *et al.*, 1994, *BioTechniques*, 17:754-761).

The present invention also encompasses antibodies conjugated to a diagnostic or therapeutic agent or any other molecule for which serum half-life is desired to be increased. The antibodies can be used diagnostically to, for example, monitor the development or progression of a disease, disorder or infection as part of a clinical testing procedure to, *e.g.*, determine the efficacy of a given treatment regimen. Detection can be facilitated by coupling the antibody to a detectable substance. Examples of detectable substances include various enzymes, prosthetic groups, fluorescent materials, luminescent materials, bioluminescent materials, radioactive materials, positron emitting metals, and nonradioactive paramagnetic metal ions. The detectable substance may be coupled or conjugated either directly to the antibody or indirectly, through an intermediate (such as, for example, a linker known in the art) using techniques known in the art. See, for example, U.S. Patent No. 4,741,900 for metal ions which can be conjugated to antibodies for use as diagnostics according to the present invention. Examples of suitable enzymes include horseradish peroxidase, alkaline phosphatase, beta-galactosidase, or acetylcholinesterase; examples of suitable prosthetic group complexes include streptavidin/biotin and avidin/biotin; examples of suitable fluorescent materials include umbelliferone, fluorescein, fluorescein isothiocyanate, rhodamine, dichlorotriazinylamine fluorescein, dansyl chloride or phycoerythrin; an example of a luminescent material includes luminol; examples of bioluminescent materials include luciferase, luciferin, and aequorin; and examples of suitable radioactive material include  $^{125}\text{I}$ ,  $^{131}\text{I}$ ,  $^{111}\text{In}$  or  $^{99}\text{Tc}$ .

An antibody may be conjugated to a therapeutic moiety such as a cytotoxin (*e.g.*, a cytostatic or cytotoxic agent), a therapeutic agent or a radioactive element (*e.g.*, alpha-emitters, gamma-emitters, etc.). Cytotoxins or cytotoxic agents include any agent that is detrimental to cells. Examples include paclitaxol, cytochalasin B, gramicidin D, ethidium bromide, emetine, mitomycin, etoposide, tenoposide, vincristine, vinblastine, colchicin, doxorubicin, daunorubicin, dihydroxy anthracin dione, mitoxantrone, mithramycin, actinomycin D, 1-dehydrotestosterone, glucocorticoids, procaine, tetracaine, lidocaine,



propranolol, and puromycin and analogs or homologs thereof. Therapeutic agents include, but are not limited to, antimetabolites (*e.g.*, methotrexate, 6-mercaptopurine, 6-thioguanine, cytarabine, 5-fluorouracil decarbazine), alkylating agents (*e.g.*, mechlorethamine, thioepa chlorambucil, melphalan, carmustine (BSNU) and lomustine (CCNU), cyclophosphamide, busulfan, dibromomannitol, streptozotocin, mitomycin C, and cisdichlorodiamine platinum (II) (DDP) cisplatin), anthracyclines (*e.g.*, daunorubicin (formerly daunomycin) and doxorubicin), antibiotics (*e.g.*, dactinomycin (formerly actinomycin), bleomycin, mithramycin, and anthramycin (AMC)), and anti-mitotic agents (*e.g.*, vincristine and vinblastine).

Further, an antibody may be conjugated to a therapeutic agent or drug moiety that modifies a given biological response. Therapeutic agents or drug moieties are not to be construed as limited to classical chemical therapeutic agents. For example, the drug moiety may be a protein or polypeptide possessing a desired biological activity. Such proteins may include, for example, a toxin such as abrin, ricin A, pseudomonas exotoxin, or diphtheria toxin; a protein such as tumor necrosis factor,  $\alpha$ -interferon (IFN- $\alpha$ ),  $\beta$ -interferon (IFN- $\beta$ ), nerve growth factor (NGF), platelet derived growth factor (PDGF), tissue plasminogen activator (TPA), an apoptotic agent (*e.g.*, TNF- $\alpha$ , TNF- $\beta$ , AIM I as disclosed in PCT Publication No. WO 97/33899), AIM II (see, PCT Publication No. WO 97/34911), Fas Ligand (Takahashi *et al.*, 1994, *J. Immunol.*, 6:1567-1574), and VEGI (PCT Publication No. WO 99/23105), a thrombotic agent or an anti-angiogenic agent (*e.g.*, angiostatin or endostatin); or a biological response modifier such as, for example, a lymphokine (*e.g.*, interleukin-1 ("IL-1"), interleukin-2 ("IL-2"), interleukin-6 ("IL-6"), granulocyte macrophage colony stimulating factor ("GM-CSF"), and granulocyte colony stimulating factor ("G-CSF"), or a growth factor (*e.g.*, growth hormone ("GH")).

Techniques for conjugating such therapeutic moieties to antibodies are well known; see, *e.g.*, Arnon *et al.*, "Monoclonal Antibodies For Immunotargeting Of Drugs In Cancer Therapy", in *Monoclonal Antibodies And Cancer Therapy*, Reisfeld *et al.* (eds.), 1985, pp. 243-56, Alan R. Liss, Inc.); Hellstrom *et al.*, "Antibodies For Drug Delivery", in *Controlled Drug Delivery (2nd Ed.)*, Robinson *et al.* (eds.), 1987, pp. 623-53, Marcel Dekker, Inc.); Thorpe, "Antibody Carriers Of Cytotoxic Agents In Cancer Therapy: A Review", in *Monoclonal Antibodies '84: Biological And Clinical Applications*, Pinchera *et al.* (eds.), 1985, pp. 475-506); "Analysis, Results, And Future Prospective Of The Therapeutic Use Of Radiolabeled Antibody In Cancer Therapy", in *Monoclonal Antibodies For Cancer Detection And Therapy*, Baldwin *et al.* (eds.), 1985, pp. 303-16, Academic Press; and Thorpe *et al.*, 1982, *Immunol. Rev.*, 62:119-58.



An antibody or fragment thereof, with or without a therapeutic moiety conjugated to it, administered alone or in combination with cytotoxic factor(s) and/or cytokine(s) can be used as a therapeutic.

Alternatively, an antibody can be conjugated to a second antibody to form an antibody heteroconjugate as described by Segal in U.S. Patent No. 4,676,980, which is incorporated herein by reference in its entirety.

Antibodies may also be attached to solid supports, which are particularly useful for immunoassays or purification of the target antigen. Such solid supports include, but are not limited to, glass, cellulose, polyacrylamide, nylon, polystyrene, polyvinyl chloride or polypropylene.

## 5.9 Crystal Structure

### 5.9.1 Crystalline FimCH

In another aspect, the present invention provides co-crystals of FimCH complexes with a mannose sugar, the crystal structures derived therefrom and methods of their use.

In the co-crystals, the mannose sugar can be any mannose sugar including, for example, mannopentanose, methyl- $\alpha$ -D-mannopyranoside,  $\alpha$ -D-mannopyranoside, mannotriose, an oligomannoside, a dimannoside, etc.

The crystals from which the atomic structure coordinates of the invention may be obtained include native crystals and heavy-atom derivative crystals. Native crystals generally comprise substantially pure polypeptides corresponding to FimCH in crystalline form.

It is to be understood that the crystalline FimCH from which the atomic structure coordinates of the invention can be obtained is not limited to wild-type FimCH. Indeed, the crystals may comprise mutants of wild-type FimCH. Mutants of wild-type FimCH are obtained by replacing at least one amino acid residue in the sequence of the wild-type FimCH with a different amino acid residue, or by adding or deleting one or more amino acid residues within the wild-type sequence and/or at the N- and/or C-terminus of the wild-type FimCH.

The types of mutants contemplated by this invention include conservative mutants, non-conservative mutants, deletion mutants, truncated mutants, extended mutants, methionine mutants, selenomethionine mutants, cysteine mutants and selenocysteine mutants. A mutant may have, but need not have, FimCH activity. Methionine, selenomethionine, cysteine, and selenocysteine mutants are particularly useful for producing



heavy-atom derivative crystals, as described in detail, below.

It will be recognized by one of skill in the art that the types of mutants contemplated herein are not mutually exclusive; that is, for example, a polypeptide having a conservative mutation in one amino acid may in addition have several Leu or Ile to Met mutations.

The amino acid residue Cys (C) is unusual in that it can form disulfide bridges with other Cys (C) residues or other sulfhydryl-containing amino acids ("cysteine-like amino acids"). The ability of Cys (C) residues and other cysteine-like amino acids to exist in a polypeptide in either the reduced free -SH or oxidized disulfide-bridged form affects whether Cys (C) residues contribute net hydrophobic or hydrophilic character to a polypeptide. While Cys (C) exhibits a hydrophobicity of 0.29 according to the consensus scale of Eisenberg *et al.* (1984, *J. Mol. Biol.* 179:125-142.), it is to be understood that for purposes of the present invention Cys (C) is categorized as a polar hydrophilic amino acid, notwithstanding the general classifications defined above. Preferably, Cys residues that are known to participate in disulfide bridges are not substituted or are conservatively substituted with other cysteine-like amino acids so that the residue can participate in a disulfide bridge. Typical cysteine-like residues include, for example, Pen, hCys, etc. Substitutions for Cys residues that interfere with crystallization are discussed *infra*.

While in most instances the amino acids of FimCH will be substituted with genetically-encoded amino acids, in certain circumstances mutants may include genetically non-encoded amino acids. For example, non-encoded derivatives of certain encoded amino acids, such as SeMet and/or SeCys, may be incorporated into the polypeptide chain using biological expression systems (such SeMet and SeCys mutants are described in more detail, *infra*).

Alternatively, in instances where the mutant will be prepared in whole or in part by chemical synthesis, virtually any non-encoded amino acids may be used, ranging from D-isomers of the genetically encoded amino acids to non-encoded naturally-occurring natural and synthetic amino acids.

Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other non-encoded amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete from and/or add amino acid residues to FimCH in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the



polypeptide, etc. Such substitutions, deletions and/or additions that do not substantially alter the three dimensional structure of the native FimCH will be apparent to those having skills in the art. These substitutions, deletions and/or additions include, but are not limited to, His tags, intein-containing self-cleaving tags, maltose binding protein fusions, glutathione S-transferase protein fusions, antibody fusions, green fluorescent protein fusions, signal peptide fusions, biotin accepting peptide fusions, and the like.

Mutations may also be introduced into a polypeptide sequence where there are residues, *e.g.*, cysteine residues, that interfere with crystallization. Such cysteine residues can be substituted with an appropriate amino acid that does not readily form covalent bonds with other amino acid residues under crystallization conditions; *e.g.*, by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non- $\beta$ -stranded segment, based on secondary structure assignments, are good candidates for replacement.

It should be noted that the mutants contemplated herein need not exhibit FimCH activity. Indeed, amino acid substitutions, additions or deletions that interfere with the activity of FimCH are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to provide phase information to aid the determination of the three-dimensional X-ray structures of other related or non-related crystalline polypeptides.

The heavy-atom derivative crystals from which the atomic structure coordinates of the invention are obtained generally comprise a crystalline FimCH polypeptide in association with one or more heavy metal atoms. The polypeptide may correspond to a wild-type or a mutant FimCH, which may optionally be in co-complex with one or more molecules, as previously described. There are two types of heavy-atom derivatives of polypeptides: heavy-atom derivatives resulting from exposure of the protein to a heavy metal in solution, wherein crystals are grown in medium comprising the heavy metal, or in crystalline form, wherein the heavy metal diffuses into the crystal, and heavy-atom derivatives wherein the polypeptide comprises heavy-atom containing amino acids, *e.g.*, selenomethionine and/or selenocysteine mutants.

In practice, heavy-atom derivatives of the first type can be formed by soaking a native crystal in a solution comprising heavy metal atom salts, or organometallic compounds, *e.g.*, lead chloride, gold thiomalate, ethylmercurithiosalicylic acid-sodium salt (thimerosal), uranyl acetate, platinum tetrachloride, osmium tetroxide, zinc sulfate, and cobalt hexamine, which can diffuse through the crystal and bind to the crystalline polypeptide.



Heavy-atom derivatives of this type can also be formed by adding to a crystallization solution comprising the polypeptide to be crystallized an amount of a heavy metal atom salt, which may associate with the protein and be incorporated into the crystal. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the crystal. This information, in turn, is used to generate the phase information needed to construct the three-dimensional structure of the protein.

Heavy-atom derivative crystals may also be prepared from polypeptides that include one or more SeMet and/or SeCys residues (SeMet and/or SeCys mutants). Such selenocysteine or selenomethionine mutants may be made from wild-type or mutant FimCH by expression of FimCH-encoding cDNAs in auxotrophic *E. coli* strains. Hendrickson *et al.*, 1990, EMBO J. 9(5):1665-1672. In this method, the wild-type or mutant FimCH cDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both). Alternatively, selenocysteine or selenomethionine mutants may be made using nonauxotrophic *E. coli* strains, *e.g.*, by inhibiting methionine biosynthesis in these strains with high concentrations of Ile, Lys, Phe, Leu, Val or Thr and then providing selenomethionine in the medium (Doublié, 1997, *Methods in Enzymology* 276:523-530). Furthermore, selenocysteine can be selectively incorporated into polypeptides by exploiting the prokaryotic and eukaryotic mechanisms for selenocysteine incorporation into certain classes of proteins *in vivo*, as described in U.S. Patent No. 5,700,660 to Leonard *et al.* (filed June 7, 1995). One of skill in the art will recognize that selenocysteine is preferably not incorporated in place of cysteine residues that form disulfide bridges, as these may be important for maintaining the three-dimensional structure of the protein and are preferably not to be eliminated. One of skill in the art will further recognize that, in order to obtain accurate phase information, approximately one selenium atom should be incorporated for every 140 amino acid residues of the polypeptide chain. The number of selenium atoms incorporated into the polypeptide chain can be conveniently controlled by designing a Met or Cys mutant having an appropriate number of Met and/or Cys residues, as described more fully below.

In some instances, the polypeptide to be crystallized may not contain cysteine or methionine residues. Therefore, if selenomethionine and/or selenocysteine mutants are to be used to obtain heavy-atom derivative crystals, methionine and/or cysteine residues may be introduced into the polypeptide chain. Likewise, Cys residues must be introduced into the polypeptide chain if the use of a cysteine-binding heavy metal, such as mercury, is contemplated for production of a heavy-atom derivative crystal.



Such mutations are preferably introduced into the polypeptide sequence at sites that will not disturb the overall protein fold. For example, a residue that is conserved among many members of the protein family or that is thought to be involved in maintaining its activity or structural integrity, as determined by, *e.g.*, sequence alignments, should not be mutated to a Met or Cys. In addition, conservative mutations, such as Ser to Cys, or Leu or Ile to Met, are preferably introduced. One additional consideration is that, in order for a heavy-atom derivative crystal to provide phase information for structure determination, the location of the heavy atom(s) in the crystal unit cell must be determinable and provide phase information. Therefore, a mutation is preferably not introduced into a portion of the protein that is likely to be mobile, *e.g.*, at, or within about 1-5 residues of, the – and C-termini.

Conversely, if there are too many methionine and/or cysteine residues in a polypeptide sequence, over-incorporation of the selenium-containing side chains can lead to the inability of the polypeptide to fold and/or crystallize, and may potentially lead to complications in solving the crystal structure. In this case, methionine and/or cysteine mutants are prepared by substituting one or more of these Met and/or Cys residues with another residue. The considerations for these substitutions are the same as those discussed above for mutations that introduce methionine and/or cysteine residues into the polypeptide. Specifically, the Met and/or Cys residues are preferably conservatively substituted with Leu/Ile and Ser, respectively.

As DNA encoding cysteine and methionine mutants can be used in the methods described above for obtaining SeCys and SeMet heavy-atom derivative crystals, the preferred Cys or Met mutant will have one Cys or Met residue for every 140 amino acids.

### 5.9.2 Crystallization Of Polypeptides And Characterization Of Crystals

The native, heavy-atom derivative and co-crystals from which the atomic structure coordinates of the invention are obtained can be obtained by conventional means as are well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, and vapor diffusion methods (see, *e.g.*, McPherson, 1998, 'Crystallization of Biological Macromolecules', Cold Spring Harbor Press, New York; McPherson, 1990, *Eur. J. Biochem.* 189:1-23.; Weber, 1991, *Adv. Protein Chem.* 41:1-36.).

Generally, native crystals are grown by dissolving substantially pure FimCH polypeptide complex in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Examples of precipitants include, but are not limited to, polyethylene glycol, ammonium sulfate, 2-methyl-2,4-pentanediol, sodium



citrate, sodium chloride, glycerol, isopropanol, lithium sulfate, sodium acetate, sodium formate, potassium sodium tartrate, ethanol, hexanediol, ethylene glycol, dioxane, t-butanol and combinations thereof. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

5 In a preferred embodiment, native crystals are grown by vapor diffusion in sitting drops (McPherson, 1982, "Preparation and Analysis of Protein Crystals", John Wiley, New York; McPherson, 1990, *Eur. J. Biochem.* 189:1-23). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals.

10 Generally, less than about 25  $\mu$ l of substantially pure polypeptide solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. The sealed container is allowed to stand, usually for about 2-6 weeks, until crystals grow.

In one embodiment of the invention, native co-crystals of a wild type FimCH

15 alpha-D-mannopyranoside complex from which atomic structure coordinates of the invention are obtained, can be obtained by the hanging drop method or by the sitting drop method. About 6  $\mu$ l of FimCH polypeptide (4.7 mg/ml in 100 mM Tris-HCl, pH 8.2, and 7 mM alpha-D-mannopyranoside) and 6  $\mu$ l reservoir solution (0.7 M ammonium sulfate and 100 mM Tris-HCl, pH 8.2) suspended over 0.5 ml reservoir solution for about 3 to 4 weeks

20 at 20°C provide diffraction quality crystals. The buffer solution optionally can be raised to 0.9 to 1.2 M ammonium sulfate after about two days, and the crystallization solution can be optionally microseeded with, for example, a cat whisker after one week to improve crystallization.

In another embodiment of the invention, co-crystals of a wild type FimCH

25 Q133N methyl-alpha-D-mannopyranoside complex from which atomic structure coordinates of the invention are obtained, can be obtained by the hanging drop method or by the sitting drop method. About 6  $\mu$ l of FimCH Q133N complex (4.7 mg/ml in 100 mM Tris-HCl, pH 8.2, and 10 mM methyl-alpha-D-mannopyranoside) and 6  $\mu$ l reservoir solution (0.7 M ammonium sulfate and 100 mM Tris-HCl, pH 8.2) suspended over 0.5 ml reservoir solution

30 for about 3 to 4 weeks at 20°C provide diffraction quality crystals. The buffer solution optionally can be raised to 0.9 to 1.2 M ammonium sulfate after about two days, and the crystallization solution can be optionally microseeded with, for example, a cat whisker after one week to improve crystallization.

Of course, those having skill in the art will recognize that the above-

35 described crystallization conditions can be varied. Such variations may be used alone or in



combination, and include polypeptide solutions containing polypeptide concentrations between 0.06 to 0.12 mM, alpha-D-mannopyranoside or methyl-alpha-D-mannopyranoside concentrations between 0.5 and 30 mM, Tris-HCl concentrations between 50 mM and 100 mM, pH ranges between 7.8 and 8.6; and reservoir solutions containing ammonium sulfate concentrations between 0.6 M and 1.2 M, Tris-HCl concentrations between 50 mM and 100 mM, pH ranges between 7.8 and 8.6 and temperature ranges between 18°C and 24°C. Other buffer solutions may be used such as Hepes buffer, so long as the desired pH range is maintained.

Heavy-atom derivative crystals can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. Heavy-atom derivative crystals can also be obtained from SeMet and/or SeCys mutants, as described above for native crystals.

Mutant complexes other than those discussed above may crystallize under slightly different crystallization conditions than wild-type protein, or under very different crystallization conditions, depending on the nature of the mutation, and its location in the protein. For example, a non-conservative mutation may result in alteration of the hydrophilicity of the mutant, which may in turn make the mutant protein either more soluble or less soluble than the wild-type protein. Typically, if a protein becomes more hydrophilic as a result of a mutation, it will be more soluble than the wild-type protein in an aqueous solution and a higher precipitant concentration will be needed to cause it to crystallize. Conversely, if a protein becomes less hydrophilic as a result of a mutation, it will be less soluble in an aqueous solution and a lower precipitant concentration will be needed to cause it to crystallize. If the mutation happens to be in a region of the protein involved in crystal lattice contacts, crystallization conditions may be affected in more unpredictable ways.



Co-crystals can also be obtained by soaking a native crystal in mother liquor containing compound that binds FimCH, or by co-crystallizing FimCH in the presence of one or more binding compounds, as discussed above.

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### 5.9.3 Characterization of Crystals

The dimensions of a unit cell of a crystal are defined by six numbers, the lengths of three unique edges,  $a$ ,  $b$ , and  $c$ , and three unique angles,  $\alpha$ ,  $\beta$ , and  $\gamma$ . The type of unit cell that comprises a crystal is dependent on the values of these variables, as discussed above in Section 3.2.

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When a crystal is placed in an X-ray beam, the incident X-rays interact with the electron cloud of the molecules that make up the crystal, resulting in X-ray scatter. The combination of X-ray scatter with the lattice of the crystal gives rise to nonuniformity of the scatter; areas of high intensity are called diffracted X-rays. The angle at which diffracted beams emerge from the crystal can be computed by treating diffraction as if it were reflection from sets of equivalent, parallel planes of atoms in a crystal (Bragg's Law). The most obvious sets of planes in a crystal lattice are those that are parallel to the faces of the unit cell. These and other sets of planes can be drawn through the lattice points. Each set of planes is identified by three indices,  $hkl$ . The  $h$  index gives the number of parts into which the  $a$  edge of the unit cell is cut, the  $k$  index gives the number of parts into which the  $b$  edge of the unit cell is cut, and the  $l$  index gives the number of parts into which the  $c$  edge of the unit cell is cut by the set of  $hkl$  planes. Thus, for example, the 235 planes cut the  $a$  edge of each unit cell into halves, the  $b$  edge of each unit cell into thirds, and the  $c$  edge of each unit cell into fifths. Planes that are parallel to the  $bc$  face of the unit cell are the 100 planes; planes that are parallel to the  $ac$  face of the unit cell are the 010 planes; and planes that are parallel to the  $ab$  face of the unit cell are the 001 planes.

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When a detector is placed in the path of the diffracted X-rays, in effect cutting into the sphere of diffraction, a series of spots, or reflections, are recorded to produce a "still" diffraction pattern. Each reflection is the result of X-rays reflecting off one set of parallel planes, and is characterized by an intensity, which is related to the distribution of molecules in the unit cell, and  $hkl$  indices, which correspond to the parallel planes from which the beam producing that spot was reflected. If the crystal is rotated about an axis perpendicular to the X-ray beam, a large number of reflections is recorded on the detector, resulting in a diffraction pattern.

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The unit cell dimensions and space group of a crystal can be determined from its diffraction pattern. First, the spacing of reflections is inversely proportional to the



lengths of the edges of the unit cell. Therefore, if a diffraction pattern is recorded when the X-ray beam is perpendicular to a face of the unit cell, two of the unit cell dimensions may be deduced from the spacing of the reflections in the x and y directions of the detector, the crystal-to-detector distance, and the wavelength of the X-rays. Those of skill in the art will appreciate that, in order to obtain all three unit cell dimensions, the crystal must be rotated such that the X-ray beam is perpendicular to another face of the unit cell. Second, the angles of a unit cell can be determined by the angles between lines of spots on the diffraction pattern. Third, the absence of certain reflections and the repetitive nature of the diffraction pattern, which may be evident by visual inspection, indicate the internal symmetry, or space group, of the crystal. Therefore, a crystal may be characterized by its unit cell and space group, as well as by its diffraction pattern.

Once the dimensions of the unit cell are determined, the likely number of polypeptides in the asymmetric unit can be deduced from the size of the polypeptide, the density of the average protein, and the typical solvent content of a protein crystal, which is usually in the range of 30-70% of the unit cell volume (Matthews, 1968, *J. Mol. Biol.* 33:491-497).

The FimCH crystals of the present invention are generally characterized by a diffraction pattern. The crystals are further characterized by unit cell dimensions and space group symmetry information obtained from the diffraction patterns, as described above. The wild type FimCH alpha-D-mannopyranoside co-crystals and the FimCH Q133N methyl-alpha-D-mannopyranoside co-crystals, have a c-centered monoclinic unit cell and space group symmetry C2.

Several forms of crystalline FimCH were obtained. In the wild type FimCH alpha-D-mannopyranoside co-crystals, the unit cell has dimensions of  $a=138.077\pm0.2$  Å,  $b=138.130\pm0.2$  Å,  $c=215.352\pm0.2$  Å,  $\alpha=90$ ,  $\beta=90.005$ ,  $\gamma=90$ . In the FimCH Q133N methyl-alpha-D-mannopyranoside co-crystals, the unit cell has dimensions of  $a=138.35\pm0.2$  Å,  $b=138.334\pm0.2$  Å,  $c=213.212\pm0.2$  Å and  $\beta=89.983^\circ\pm0.2^\circ$ . There are likely to be 8 FimCH molecules in the asymmetric unit in both crystalline forms, related by an approximate four-fold axis.

#### **5.9.4 Collection of Data and Determination of Structure Solutions**

The diffraction pattern is related to the three-dimensional shape of the molecule by a Fourier transform. The process of determining the solution is in essence a re-focusing of the diffracted X-rays to produce a three-dimensional image of the molecule in



the crystal. Since re-focusing of X-rays cannot be done with a lens at this time, it is done via mathematical operations.

5 The sphere of diffraction has symmetry that depends on the internal symmetry of the crystal, which means that certain orientations of the crystal will produce the same set of reflections. Thus, a crystal with high symmetry has a more repetitive diffraction pattern, and there are fewer unique reflections that need to be recorded in order to have a complete representation of the diffraction. The goal of data collection, a data set, is a set of consistently measured, indexed intensities for as many reflections as possible. A complete data set is collected if at least 80%, preferably at least 90%, most preferably at least 95% of  
10 unique reflections are recorded. In one embodiment, a complete data set is collected using one crystal. In another embodiment, a complete data set is collected using more than one crystal of the same type.

Sources of X-rays include, but are not limited to, a rotating anode X-ray generator such as a Rigaku RU-200 or a beamline at a synchrotron light source, such as the  
15 Advanced Photon Source at Argonne National Laboratory. Suitable detectors for recording diffraction patterns include, but are not limited to, X-ray sensitive film, multiwire area detectors, image plates coated with phosphorus, and CCD cameras. Typically, the detector and the X-ray beam remain stationary, so that, in order to record diffraction from different parts of the crystal's sphere of diffraction, the crystal itself is moved via an automated  
20 system of moveable circles called a goniostat.

One of the biggest problems in data collection, particularly from macromolecular crystals having a high solvent content, is the rapid degradation of the crystal in the X-ray beam. In order to slow the degradation, data is often collected from a crystal at liquid nitrogen temperatures. In order for a crystal to survive the initial exposure to liquid  
25 nitrogen, the formation of ice within the crystal must be prevented by the use of a cryoprotectant. Suitable cryoprotectants include, but are not limited to, low molecular weight polyethylene glycols, ethylene glycol, sucrose, glycerol, xylitol, and combinations thereof. Crystals may be soaked in a solution comprising the one or more cryoprotectants prior to exposure to liquid nitrogen, or the one or more cryoprotectants may be added to the  
30 crystallization solution. Data collection at liquid nitrogen temperatures may allow the collection of an entire data set from one crystal.

Once a data set is collected, the information is used to determine the three-dimensional structure of the molecule in the crystal. However, this cannot be done from a single measurement of reflection intensities because certain information, known as phase  
35 information, is lost between the three-dimensional shape of the molecule and its Fourier



transform, the diffraction pattern. This phase information must be acquired by methods described below in order to perform a Fourier transform on the diffraction pattern to obtain the three-dimensional structure of the molecule in the crystal. It is the determination of phase information that in effect refocuses X-rays to produce the image of the molecule.

5 One method of obtaining phase information is by isomorphous replacement, in which heavy-atom derivative crystals are used. In this method, the positions of heavy atoms bound to the molecules in the heavy-atom derivative crystal are determined, and this information is then used to obtain the phase information necessary to elucidate the three-dimensional structure of a native crystal. (Blundel *et al.*, 1976, Protein Crystallography,  
10 Academic Press).

Another method of obtaining phase information is by molecular replacement, which is a method of calculating initial phases for a new crystal of a polypeptide whose structure coordinates are unknown by orienting and positioning a polypeptide whose structure coordinates are known within the unit cell of the new crystal so as to best account  
15 for the observed diffraction pattern of the new crystal. Phases are then calculated from the oriented and positioned polypeptide and combined with observed amplitudes to provide an approximate Fourier synthesis of the structure of the molecules comprising the new crystal. (Lattman, 1985, *Methods in Enzymology* 115:55-77; Rossmann, 1972, "The Molecular Replacement Method," Int. Sci. Rev. Ser. No. 13, Gordon & Breach, New York).

20 A third method of phase determination is multi-wavelength anomalous diffraction or MAD. In this method, X-ray diffraction data are collected at several different wavelengths from a single crystal containing at least one heavy atom with absorption edges near the energy of incoming X-ray radiation. The resonance between X-rays and electron orbitals leads to differences in X-ray scattering that permits the locations of the heavy atoms  
25 to be identified, which in turn provides phase information for a crystal of a polypeptide. A detailed discussion of MAD analysis can be found in Hendrickson, 1985, *Trans. Am. Crystallogr. Assoc.*, 21:11; Hendrickson *et al.*, 1990, *EMBO J.* 9:1665; and Hendrickson, 1991, *Science* 4:91.

30 A fourth method of determining phase information is single wavelength anomalous dispersion or SAD. In this technique, X-ray diffraction data are collected at a single wavelength from a single native or heavy-atom derivative crystal, and phase information is extracted using anomalous scattering information from atoms such as sulfur or chlorine in the native crystal or from the heavy atoms in the heavy-atom derivative crystal. The wavelength of X-rays used to collect data for this phasing technique need not  
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be close to the absorption edge of the anomalous scatterer. A detailed discussion of SAD analysis can be found in Brodersen *et al.*, 2000, *Acta Cryst.*, D56:431-441.

A fifth method of determining phase information is single isomorphous replacement with anomalous scattering or SIRAS. This technique combines isomorphous replacement and anomalous scattering techniques to provide phase information for a crystal of a polypeptide. X-ray diffraction data are collected at a single wavelength, usually from a single heavy-atom derivative crystal. Phase information obtained only from the location of the heavy atoms in a single heavy-atom derivative crystal leads to an ambiguity in the phase angle, which is resolved using anomalous scattering from the heavy atoms. Phase information is therefore extracted from both the location of the heavy atoms and from anomalous scattering of the heavy atoms. A detailed discussion of SIRAS analysis can be found in North, 1965, *Acta Cryst.* 18:212-216; Matthews, 1966, *Acta Cryst.* 20:82-86.

Once phase information is obtained, it is combined with the diffraction data to produce an electron density map, an image of the electron clouds that surround the molecules in the unit cell. The higher the resolution of the data, the more distinguishable are the features of the electron density map, *e.g.*, amino acid side chains and the positions of carbonyl oxygen atoms in the peptide backbones, because atoms that are closer together are resolvable. A model of the macromolecule is then built into the electron density map with the aid of a computer, using as a guide all available information, such as the polypeptide sequence and the established rules of molecular structure and stereochemistry. Interpreting the electron density map is a process of finding the chemically reasonable conformation that fits the map precisely.

After a model is generated, a structure is refined. Refinement is the process of minimizing the function  $\Phi$ , which is the difference between observed and calculated intensity values (measured by an R-factor), and which is a function of the position, temperature factor, and occupancy of each non-hydrogen atom in the model. This usually involves alternate cycles of real space refinement, *i.e.*, calculation of electron density maps and model building, and reciprocal space refinement, *i.e.*, computational attempts to improve the agreement between the original intensity data and intensity data generated from each successive model. Refinement ends when the function  $\Phi$  converges on a minimum wherein the model fits the electron density map and is stereochemically and conformationally reasonable. During refinement, ordered solvent molecules are added to the structure.

#### 5.9.4.1 Structures of FimCH



The present invention provides, for the first time, the high-resolution three-dimensional structures and atomic structure coordinates of crystalline FimCH bound to  $\alpha$ -D-mannose as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the example, *infra*. The atomic structure coordinates of crystalline wild type FimCH -  $\alpha$ -D-mannopyranoside to 2.8 Å resolution are listed in Table 14. The atomic structure coordinates of crystalline FimCH Q133N -  $\alpha$ -D-mannopyranoside to 3 Å resolution are listed in Table 15.

Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of FimCH, whether native crystals, heavy-atom derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 2 Å when superimposed, using backbone atoms (N, C $\alpha$ , C and O), on the structure coordinates listed in Table 14 are considered to be identical with the structure coordinates listed in the Table when at least about 50% to 100% of the backbone atoms of FimCH are included in the superposition.

#### 5.9.5 Structure Coordinates

The atomic structure coordinates can be used in molecular modeling and design, as described more fully below. The present invention encompasses the structure coordinates and other information, *e.g.*, amino acid sequence, connectivity tables, vector-based representations, temperature factors, etc., used to generate the three-dimensional structure of the polypeptide for use in the software programs described below and other software programs.

The invention encompasses machine readable media embedded with the three-dimensional structure of the model described herein, or with portions thereof. As used herein, "machine readable medium" refers to any medium that can be read and accessed directly by a computer or scanner. Such media include, but are not limited to: magnetic storage media, such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM or ROM; and hybrids of these categories such as magnetic/optical storage media. Such media further include paper on which is recorded a representation of the atomic structure coordinates, *e.g.*, Cartesian coordinates, that can be read by a scanning device and converted into a three-dimensional structure with an OCR.

A variety of data storage structures are available to a skilled artisan for creating a computer readable medium having recorded thereon the atomic structure



coordinates of the invention or portions thereof and/or X-ray diffraction data. The choice of the data storage structure will generally be based on the means chosen to access the stored information. In addition, a variety of data processor programs and formats can be used to store the sequence and X-ray data information on a computer readable medium. Such  
5 formats include, but are not limited to, Protein Data Bank ("PDB") format (Research Collaboratory for Structural Bioinformatics; [http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2\\_frame.html](http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html)); Cambridge Crystallographic Data Centre format ([http://www.ccdc.cam.ac.uk/support/csd\\_doc/volume3/z323.html](http://www.ccdc.cam.ac.uk/support/csd_doc/volume3/z323.html)); Structure-data ("SD")  
10 file format (MDL Information Systems, Inc.; Dalby *et al.*, 1992, *J. Chem. Inf. Comp. Sci.* 32:244-255), and line-notation, *e.g.*, as used in SMILES (Weininger, 1988, *J. Chem. Inf. Comp. Sci.* 28:31-36). Methods of converting between various formats read by different computer software will be readily apparent to those of skill in the art, *e.g.*, BABEL (v. 1.06, Walters & Stahl, ©1992, 1993, 1994;  
15 <http://www.brunel.ac.uk/departments/chem/babel.htm>). All format representations of the polypeptide coordinates described herein, or portions thereof, are contemplated by the present invention. By providing computer readable medium having stored thereon the atomic coordinates of the invention, one of skill in the art can routinely access the atomic coordinates of the invention, or portions thereof, and related information for use in modeling  
20 and design programs, described in detail below.

While Cartesian coordinates are important and convenient representations of the three-dimensional structure of a polypeptide, those of skill in the art will readily recognize that other representations of the structure are also useful. Therefore, the three-dimensional structure of a polypeptide, as discussed herein, includes not only the Cartesian  
25 coordinate representation, but also all alternative representations of the three-dimensional distribution of atoms. For example, atomic coordinates may be represented as a Z-matrix, wherein a first atom of the protein is chosen, a second atom is placed at a defined distance from the first atom, a third atom is placed at a defined distance from the second atom so that it makes a defined angle with the first atom. Each subsequent atom is placed at a defined  
30 distance from a previously placed atom with a specified angle with respect to the third atom, and at a specified torsion angle with respect to a fourth atom. Atomic coordinates may also be represented as a Patterson function, wherein all interatomic vectors are drawn and are then placed with their tails at the origin. This representation is particularly useful for locating heavy atoms in a unit cell. In addition, atomic coordinates may be represented as a  
35 series of vectors having magnitude and direction and drawn from a chosen origin to each



atom in the polypeptide structure. Furthermore, the positions of atoms in a three-dimensional structure may be represented as fractions of the unit cell (fractional coordinates), or in spherical polar coordinates.

Additional information, such as thermal parameters, which measure the motion of each atom in the structure, chain identifiers, which identify the particular chain of a multi-chain protein in which an atom is located, and connectivity information, which indicates to which atoms a particular atom is bonded, is also useful for representing a three-dimensional molecular structure.

#### 5.9.6 Uses of the Atomic Structure Coordinates

Structure information, typically in the form of the atomic structure coordinates, can be used in a variety of computational or computer-based methods to, for example, design, screen for and/or identify compounds that bind the crystallized polypeptide or a portion or fragment thereof, or to intelligently design mutants that have altered biological properties.

In one embodiment, the crystals and structure coordinates obtained therefrom are useful for identifying and/or designing compounds that bind FimC, FimH, FimCH, or a fragment thereof, as an approach towards developing new therapeutic agents. For example, a high resolution X-ray structure will often show the locations of ordered solvent molecules around the protein, and in particular at or near putative binding sites on the protein. This information can then be used to design molecules that bind these sites, the compounds synthesized and tested for binding in biological assays. Travis, 1993, Science 262:1374.

In another embodiment, the structure can be probed with a plurality of molecules to determine their ability to bind to FimC, FimH, FimCH, or a fragment thereof, at various sites. Such compounds can be used as targets or leads in medicinal chemistry efforts to identify, for example, inhibitors of potential therapeutic importance. For example, the structure coordinates can be used to identify compounds that inhibit mannose binding by FimCH. Such compounds can be used, for example, to treat or prevent urinary tract infection by a pathogen expressing FimC, FimH or FimCH.

In yet another embodiment, the structure can be used to computationally screen small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to FimC, FimH, FimCH, or a fragment thereof. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng *et al.*, 1992, J. Comp. Chem. 13:505-524.



The design of compounds that bind to FimC, FimH, FimCH, or a fragment thereof, according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with FimC, FimH, FimCH, or a fragment thereof. This association can be covalent or non-covalent. For  
5 example, covalent interactions may be important for designing irreversible inhibitors of a protein. Non-covalent molecular interactions important in the association of FimC, FimH, FimCH, or a fragment thereof, with its substrate include hydrogen bonding, ionic interactions and van der Waals and hydrophobic interactions. Second, the compound must be able to assume a conformation that allows it to associate with FimC, FimH, FimCH, or a  
10 fragment thereof. Although certain portions of the compound will not directly participate in this association with FimC, FimH, FimCH, or a fragment thereof, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical group or compound in relation to all or a portion of  
15 the binding site, or the spacing between functional groups of a compound comprising several chemical groups that directly interact with FimC, FimH, FimCH, or a fragment thereof].

The potential inhibitory or binding effect of a chemical compound on FimC, FimH, FimCH, or a fragment thereof, may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given  
20 compound suggests insufficient interaction and association between it and FimC, FimH, FimCH, or a fragment thereof, synthesis and testing of the compound is unnecessary. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to FimC, FimH, FimCH, or a fragment thereof, and inhibit its activity. In this manner, synthesis of ineffective compounds may be avoided.

25 An inhibitory or other binding compound of FimC, FimH, FimCH, or a fragment thereof, may be computationally evaluated and designed by means of a series of steps in which chemical groups or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of FimC, FimH, FimCH, or a fragment thereof. One skilled in the art may use one of several methods to screen chemical  
30 groups or fragments for their ability to associate with FimC, FimH, FimCH, or a fragment thereof. This process may begin by visual inspection of, for example, the active site on the computer screen based on the coordinates of FimC, FimH, FimCH, or a fragment thereof. Selected fragments or chemical groups may then be positioned in a variety of orientations, or docked, within an individual binding pocket of FimC, FimH, FimCH, or a fragment thereof,  
35 as defined supra. Docking may be accomplished using software such as QUANTA and



SYBYL, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical groups. These include:

- 5       1.     GRID (Goodford, 1985, J. Med. Chem. 28:849-857). GRID is available from Oxford University, Oxford, UK;
2.     MCSS (Miranker & Karplus, 1991, Proteins: Structure, Function and Genetics 11:29-34). MCSS is available from Molecular Simulations, Burlington, MA;
- 10     3.     AUTODOCK (Goodsell & Olsen, 1990, Proteins: Structure, Function, and Genetics 8:195-202). AUTODOCK is available from Scripps Research Institute, La Jolla, CA; and
4.     DOCK (Kuntz *et al.*, 1982, J. Mol. Biol. 161:269-288). DOCK is available from University of California, San Francisco, CA.

15       Once suitable chemical groups or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may proceed by visual inspection of the relationship of the fragments to each other in the three-dimensional image displayed on a computer screen in relation to the structure coordinates of FimC, FimH, FimCH, or a fragment thereof. This would be followed by manual model building using software such as QUANTA or SYBYL.

20       Useful programs to aid one of skill in the art in connecting the individual chemical groups or fragments include:

- 25     1.     CAVEAT (Bartlett *et al.*, 1989, 'CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules'. In Molecular Recognition in Chemical and Biological Problems', Special Pub., Royal Chem. Soc. 78:182-196). CAVEAT is available from the University of California, Berkeley, CA;
2.     3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Martin, 1992, J. Med. Chem. 35:2145-2154); and
3.     HOOK (available from Molecular Simulations, Burlington, Mass.).

30       Instead of proceeding to build an inhibitor of FimC, FimH, FimCH, or a fragment thereof, in a step-wise fashion one fragment or chemical group at a time, as described above, compounds that bind may be designed as a whole or 'de novo' using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include:

- 35     1.     LUDI (Bohm, 1992, J. Comp. Aid. Molec. Design 6:61-78). LUDI is available from Molecular Simulations, Inc., San Diego, CA;



2. LEGEND (Nishibata & Itai, 1991, Tetrahedron 47:8985). LEGEND is available from Molecular Simulations, Burlington, Mass.; and

3. LeapFrog (available from Tripos, Inc., St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. *See, e.g.,* Cohen *et al.*, 1990, J. Med. Chem. 33:883-894. *See also,* Navia & Murcko, 1992, Current Opinions in Structural Biology 2:202-210.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to FimC, FimH, FimCH, or a fragment thereof, may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as an inhibitor of FimC, FimH, FimCH, or a fragment thereof, must also preferably occupy a volume not overlapping the volume occupied by the active site residues when the native substrate is bound. An effective inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (*i.e.*, it must have a small deformation energy of binding). Thus, the most efficient inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mol, preferably, not greater than 7 kcal/mol. Inhibitors may interact with the protein in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the enzyme.

A compound selected or designed for binding to FimC, FimH, FimCH, or a fragment thereof, may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target protein. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the protein when the inhibitor is bound to it preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C (Frisch, Gaussian, Inc., Pittsburgh, PA, ©1992); AMBER, version 4.0 (Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA, ©1994); and Insight II/Discover (Biosym Technologies Inc., San Diego, CA, ©1994). These programs may be implemented, for instance, using a computer workstation, as are well-known in the art. Other hardware systems and software packages will be known to those skilled in the art.



Once a binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or chemical groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, *i.e.*, the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. One of skill in the art will understand that substitutions known in the art to alter conformation should be avoided. Such altered chemical compounds may then be analyzed for efficiency of binding to FimC, FimH, FimCH, or a fragment thereof, by the same computer methods described in detail above.

Because FimC, FimH, FimCH, or a fragment thereof, may crystallize in more than one crystal form, the structure coordinates of FimC, FimH, FimCH, or a fragment thereof, are particularly useful to solve the structure of those other crystal forms of FimC, FimH, FimCH, or a fragment thereof. They may also be used to solve the structure of mutants, co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of FimC, FimH or FimCH.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of FimC, FimH, FimCH, or a fragment thereof, a mutant, or a co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of FimC, FimH or FimCH, may be determined using phase information from the structure coordinates. This method may provide an accurate three-dimensional structure for the unknown protein in the new crystal more quickly and efficiently than attempting to determine such information *ab initio*. In addition, in accordance with this invention, mutants may be crystallized in co-complex with known inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type FimC, FimH, FimCH, or a fragment thereof. Potential sites for modification within the various binding sites of the protein may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between FimC, FimH, FimCH, or a fragment thereof, and a chemical group or compound.

If an unknown crystal form has the same space group as and similar cell dimensions to the known FimC, FimH or FimCH crystal form, then the phases derived from the known crystal form can be directly applied to the unknown crystal form, and in turn, an electron density map for the unknown crystal form can be calculated. Difference electron density maps can then be used to examine the differences between the unknown crystal form and the known crystal form. A difference electron density map is a subtraction of one



electron density map, *e.g.*, that derived from the known crystal form, from another electron density map, *e.g.*, that derived from the unknown crystal form. Therefore, all similar features of the two electron density maps are eliminated in the subtraction and only the differences between the two structures remain. For example, if the unknown crystal form is of a co-complex, then a difference electron density map between this map and the map derived from the native, uncomplexed crystal will ideally show only the electron density of the ligand. Similarly, if amino acid side chains have different conformations in the two crystal forms, then those differences will be highlighted by peaks (positive electron density) and valleys (negative electron density) in the difference electron density map, making the differences between the two crystal forms easy to detect. However, if the space groups and/or cell dimensions of the two crystal forms are different, then this approach will not work and molecular replacement must be used in order to derive phases for the unknown crystal form.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 50 Å to 1.5 Å or greater resolution X-ray data to an R value of about 0.20 or less using computer software, such as CNS (Yale University, (c) 1992, distributed by Molecular Simulations, Inc.). See, *e.g.*, Blundel *et al.*, 1976, Protein Crystallography, Academic Press.; Methods in Enzymology, vol. 114 & 115, Wyckoff *et al.*, eds., Academic Press, 1985. This information may thus be used to optimize known classes of inhibitors, and more importantly, to design and synthesize novel classes of inhibitors.

The structure coordinates of mutants will also facilitate the identification of related proteins or enzymes analogous to FimC, FimH, FimCH, or a fragment thereof, in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing FimC, FimH or FimCH, mediated diseases.

Subsets of the atomic structure coordinates can be used in any of the above methods. Particularly useful subsets of the coordinates include, but are not limited to, coordinates of single domains, coordinates of residues lining an active site, coordinates of residues that participate in important protein-protein contacts at an interface, and C $\alpha$  coordinates. For example, the coordinates of one domain of a protein that contains the active site may be used to design inhibitors that bind to that site, even though the protein is fully described by a larger set of atomic coordinates. Therefore, a set of atomic coordinates that define the entire polypeptide chain, although useful for many applications, do not necessarily need to be used for the methods described herein.



In carrying out the procedures of the present invention it is of course to be understood that reference to particular buffers, media, reagents, cells, culture conditions and the like are not intended to be limiting, but are to be read so as to include all related materials that one of ordinary skill in the art would recognize as being of interest or value in the particular context in which that discussion is presented. For example, it is often possible to substitute one buffer system or culture medium for another and still achieve similar, if not identical, results. Those of skill in the art will have sufficient knowledge of such systems and methodologies so as to be able, without undue experimentation, to make such substitutions as will optimally serve their purposes in using the methods and procedures disclosed herein.

All publications, patents and patent applications mentioned in this specification are herein incorporated by reference into the specification to the same extent as if each individual publication, patent or patent application was specifically and individually indicated to be incorporated herein by reference.

The present invention will now be further described by way of the following non-limiting examples. In applying the disclosure of these examples, it should be kept clearly in mind that other and different embodiments of the methods disclosed according to the present invention will no doubt suggest themselves to those of skill in the relevant art.

## 6. EXAMPLES

### 6.1 EXAMPLE 1: Characterization of FimH mutants

Based on the crystal structure (Figure 2) of vaccine quality FimCH bound to mono-mannose, the mannose-binding domain on FimH was identified. This domain was in a canyon on the surface of the protein. Furthermore, some of the specific amino acids on FimH mediating the interaction with mannose were identified. A hydrophobic ring around the mannose-binding pocket was also identified. To probe critical structural and conformational requirements of FimH, the crystal structure was used to provide several candidate residues for mutation. The serine at position 62 was mutated to an alanine and used as a control since it does not lay within the pocket or the hydrophobic ring region.

#### 6.1.1 Expression and Isolation of FimCH mutants

Site specific mutations in FimH (see Table 7) were made according to techniques known in the art. A two-step PCR protocol as described for the mutagenesis of *papD* (Hung *et al.*, 1999, *Proc. Natl. Acad. Sci. USA* 96:8178-83) was used. The following



primers were used to amplify and introduce mutations in the first half of the FimH gene (\* = coding strand; # = noncoding strand):

5	EcoRI	*5'-GGGGGGAATTCACCCGGAGGGATGATTGTA-3' (SEQ ID NO:5)
	XcmI	#5'-CCAGTAGGCACCACCACATCATTATTGG-3' (SEQ ID NO:6)
10	F1A	*5'-CTGGTCGGTAAATGCCTGGTCAGCGGCCTGTAAAACCGCCAATGGTAC-3' (SEQ ID NO:7)
		#5'-GTACCATTGGCGGTTTTACAGGCCGCTGACCAGGCATTACCGACCAG-3' (SEQ ID NO:8)
15	II3A	*5'-GCCAATGGTACCGCTATCCCTGCGGGCGGTGGCAGCGCCAATG-3' (SEQ ID NO:9)
		#5'-CATTGGCGCTGCCACCGCCCGCAGGGATAGCGGTACCATTGGC-3' (SEQ ID NO:10)
20	I52A	*5'-CCATAACGATTATCCGGAAACCGCGACAGACTATGTCACACTGC-3' (SEQ ID NO:11)
		#5'-GCAGTGTGACATAGTCTGTCGCGGTTTCCGGATAATCGTTATGG-3' (SEQ ID NO:12)
25	S62A	*5'-GCAACGAGGCGCCGCTTATGGCGG-3' (SEQ ID NO:13)
		#5'-CCGCCATAAGCGGCGCCTCGTTGC-3' (SEQ ID NO:14)
30	N46A	*5'-CTTTTGCCATGCTGATTATCCGGAAACC-3' (SEQ ID NO:15)
		#5'-GGTTTCCGGATAATCAGCATGGCAAAAC-3' (SEQ ID NO:16)
35	N46D	*5'-CTTTTGCCATGATGATTATCCGGAAACC-3' (SEQ ID NO:17)
		#5'-GGTTTCCGGATAATCATCATGGCAAAAC-3' (SEQ ID NO:18)
	Y48A	*5'-GCAAATCTTTTGCCATAACGATGCGCCGGAAACCATTACAGACTATGTCACACTG-3' (SEQ ID NO:19)
		#5'-CAGTGTGACATAGTCTGTAATGGTTTCCGGCGCATCGTTATGGCAAAAGATTTGC-3' (SEQ ID NO:20)



- D54A      \*5'-ACCATTACAGCTTATGTCACACTG-3' (SEQ ID NO:21)  
#5'-CAGTGTGACATAAGCTGTAATGGT-3' (SEQ ID NO:22)
- 5      D54N      \*5'-ACCATTACAACTATGTCACACTG-3' (SEQ ID NO:23)  
#5'-CAGTGTGACATAGTTTGTAAATGGT-3' (SEQ ID NO:24)
- Q133A      \*5'-CTTATTTTGC GCGCTACCAACAAC-3' (SEQ ID NO:25)  
#5'-GTTGTTGGTAGCGCGCAAAATAAG-3' (SEQ ID NO:26)
- 10      Q133N      \*5'-CTTATTTTGC GAAATACCAACAAC-3' (SEQ ID NO:27)  
#5'-GTTGTTGGTATTTGCGCAAAATAAG-3' (SEQ ID NO:28)
- Q133K      \*5'-CTTATTTTGC GGAAGACCAACAAC-3' (SEQ ID NO:29)  
#5'-GTTGTTGGTCTTCCGCAAAATAAG-3' (SEQ ID NO:30)
- 15      Q133E      \*5'-GCCGTGCTTATTTTGC GAGAAACCAACA ACTATAACAGCGATG-3'  
(SEQ ID NO:31)  
#5'-CATCGCTGTTATAGTTGTTGGTTTCTCGCAAAATAAGCACGGC-3'  
(SEQ ID NO:32)
- 20      Q133R      \*5'-GCCGTGCTTATTTTGC GACGCACCAACA ACTATAACAGCGATG-3'  
(SEQ ID NO:33)  
#5'-CATCGCTGTTATAGTTGTTGGTGC GTCGCAAAATAAGCACGGC-3'  
(SEQ ID NO:34)
- 25      Q133H      \*5'-GCCGTGCTTATTTTGC GACATACCAACA ACTATAACAGCGATG-3'  
(SEQ ID NO:35)  
#5'-CATCGCTGTTATAGTTGTTGGTATGTCGCAAAATAAGCACGGC-3'  
(SEQ ID NO:36)
- 30      N135A      \*5'-GCGACAGACGGCCA ACTATAACAGC-3' (SEQ ID NO:37)  
#5'-GCTGTTATAGTTGGCCGTCTGTCGC-3' (SEQ ID NO:38)
- 35      N135D      \*5'-GCGACAGACCGATA ACTATAACAGC-3' (SEQ ID NO:39)  
#5'-GCTGTTATAGTTSTCGGTCTGTCGC-3' (SEQ ID NO:40)



Y137A      \*5'-GCGACAGACCAACAACGCGAACAGCGATGATTTCCAGTTTGTG-3'  
               (SEQ ID NO:41)  
               #5'-CACAACTGGAAATCATCGCTGTTTCGCGTTGTTGGTCTGTCTCGC-3'  
               (SEQ ID NO:42)

5

D140A      \*5'-CTATAACAGTGCAGATTTCCAG-3' (SEQ ID NO:43)  
               #5'-CTGGAAATCTGCACTGTTATAG-3' (SEQ ID NO:44)

D140N      \*5'-CTATAACAGCAATGATTTCCAG-3' (SEQ ID NO:45)  
               #5'-CTGGAAATCATTGCTGTTATAG-3' (SEQ ID NO:46)

10

D140E      \*5'-CTATAACAGCGAAGACTTCCAG-3' (SEQ ID NO:47)  
               #5'-CTGGAAGTCTTCGCTGTTATAG-3' (SEQ ID NO:48)

15    F142A      \*5'-GCGACAGACCAACAACACTATAACAGCGATGATGCGCAGTTTGTG-3'  
               (SEQ ID NO:49)  
               #5'-CACAACTGCGCATCATCGCTGTTATAGTTGTTGGTCTGTCTCGC-3'  
               (SEQ ID NO:50)

20

EcoR I and Xcm I restriction sites were engineered into the 5' and 3' primers, respectively for cloning. The PCR inserts were cloned into an EcoR1 and Xcm1 digested pHACW18 to generate a full-length FimH gene containing the desired mutations. Mutations in FimH were confirmed by sequencing. Each mutant was subcloned as an EcoR I-BamH I full-length FimH gene into the IPTG-inducible expression vector, pMMB66 (Furste *et al.*, 1986, *Gene* 48:119-31). The resulting plasmids, pHACWF1A, pHACWI13A, pHACWY48A, pHACWI52A, pHACWS62A, pHACWN46A, pHACWN46D, pHACWD54A, pHACWD54N, pHACWQ133A, pHACWQ133N, pHACWQ133K, pHACWQ133E, pHACWQ133R, pHACWQ133H, pHACWN135A, pHACWN135D, pHACWY137A, pHACWD140A, pHACWD140N, pHACWD140E, pHACWF142A  
 25    encode FimH with point mutations changing Phe-1 to Ala; Ile-13 to Ala; Tyr-48 to Ala; Ile-52 to Ala; Ser-62 to Ala; Asn-46 to Ala or Asp; Asp-54 to Ala or Asn; Gln-133 to Ala, Asn, Lys, Glu, Arg, or His; Asn-135 to Ala or Asp; Tyr-137 to Ala; Asp140 to Ala, Asn, or Glu; and Phe-142 to Ala. Additionally, the FimH gene may be cloned into the pCGA139-1-1  
 30    vector (see Section 5.6) for expression. The wild type FimH gene from pHACW18 was also  
 35    cloned into pMMB66 in the similar manner and designated as pHACW66. The original



pMMB66 expression vector was used as the negative control plasmid for FimH expression. All plasmids were transformed into *E. coli* strains ORN103/pUT2002, AAEC185/pUT2002, C600/pHJ9205, and K12.

Wild type FimCH is made up of an ~ 52 kDa complex composed of two wild type proteins; FimC (22.8 kDa) and FimH (29.1 kDa) in a 1:1 equimolar ratio. Periplasmic extracts were isolated as described (Slonim et al, 1992, *EMBO J.* 11:4747-56 and Jones et al., 1993, *Proc. Natl. Acad. Sci. USA* 90:8397-8401). Bacterial strain C600/pHJ9205 or K12 transformed with FimH expression constructs was used to produce large quantities of FimH proteins. These transformants were grown in LB in the presence of 0.1% arabinose and 0.1 mM IPTG to induce FimC and FimH expression, respectively. The protocol for the purification of FimCH complexes from bacterial periplasm has been described previously and was followed in this study (Barnhart et al., 2000, *Proc. Natl. Acad. Sci. USA* 97:7709-14, incorporated herein by reference). Purified FimCH complexes were dialyzed into 20 mM MES, pH 6.8 and stored at 4 °C.

Purified recombinant FimH proteins associated with wild type FimC protein. This was assayed by ELISA using an anti-FimC antibody to detect FimCH complexes (Figure 4). Each of the mutant proteins was expressed, associated with FimC, and localized to the periplasm (data not shown).

Table 7: Site Directed Mutagenesis of FimH

residue position	wild type amino acid	engineered mutant amino acid
1	phenylalanine (F)	alanine (A)
13	isoleucine (I)	alanine (A)
46	asparagine (N)	alanine (A)
46	asparagine (N)	aspartic acid (D)
48	tyrosine (Y)	alanine (A)
52	isoleucine (I)	alanine (A)
54	aspartic acid (D)	alanine (A)
54	aspartic acid (D)	asparagine (N)
62*	serine (S)	alanine (A)
67	asparagine (N)	alanine (A)
67	asparagine (N)	aspartic acid (D)



75	aspartic acid (D)	alanine (A)
75	aspartic acid (D)	asparagine (N)
133	glutamine (Q)	alanine (A)
133	glutamine (Q)	lysine (K)
133	glutamine (Q)	asparagine (N)
133	glutamine (Q)	histidine (H)
133	glutamine (Q)	arginine (R)
133	glutamine (Q)	glutamic acid (E)
135	asparagine (N)	alanine (A)
135	asparagine (N)	aspartic acid (D)
135	asparagine (N)	lysine (K)
137	tyrosine (Y)	alanine (A)
140	aspartic acid (D)	alanine (A)
140	aspartic acid (D)	asparagine (N)
140	aspartic acid (D)	glutamic acid (E)
142	phenylalanine (F)	alanine (A)
154	glutamic acid (E)	alanine (A)
154	glutamic acid (E)	asparagine (N)
154	glutamic acid (E)	lysine (K)
156	asparagine (N)	alanine (A)
156	asparagine (N)	aspartic acid (D)
161	aspartic acid (D)	alanine (A)
161	aspartic acid (D)	asparagine (N)
161	aspartic acid (D)	glutamic acid (E)

\* control reside outside of the mannose-binding pocket and hydrophobic ring regions.

### 6.1.2 Bacterial Surface Staining of FimH Proteins

Bacterial strain AAEC185/pUT2002 contained a FimH-null type 1 pilus operon and was complemented with either wild type or each of the mutant FimH expression plasmids. These bacteria were cultured in the same manner as the ORN103/pUT2002



transformants for optimal FimH and type 1 pili expression. Overnight cultures were diluted to the same concentration (OD<sub>600</sub> 1) and 1 ml of diluted bacteria was used to immunostain for FimH on the bacterial surface. Bacterial cultures were washed once in PBS (0.12 M NaCl, 2.7 mM KCl, 10 mM phosphate, pH 7.4) and resuspended in 100 ul PBS+5% FBS containing 1:1000 dilution of anti-FimC/FimH antiserum (MedImmune Inc.). Binding of primary antibody was allowed to proceed for one hour on ice and followed by three washes with PBS. Bacterial pellets were resuspended in 100 ul of Oregon Green-conjugated goat-mouse IgG (H+L) secondary antibody diluted 1000-fold in PBS+5% FBS and incubated on ice for another hour. After incubation with secondary antibody, bacteria were washed extensively and fixed with 2% glutaraldehyde (in PBS) with 1 µg/ml Hoechst stain (Sigma) for 5 min at room temperature (RT). Bacteria were washed once again and resuspended in 100 ul PBS. Five microliters of stained bacteria were spotted on glass microscope slides and allowed to air-dry at room temperature. The staining of FimH on bacterial surfaces was visualized with an Olympus BX60 microscope system.

WT FimCH as well as all of the mutant FimCH proteins were properly localized to the pilus (although data is not shown, it is summarized in Table 8).

### **6.1.3 Mannose Binding Properties of mutant FimCH proteins**

FimH allelic variants can be broadly divided into two functional groups, those that bind tri-mannose only and those that also are capable of binding mono-mannose. Mono-mannose binding activity has been correlated to an increased virulence phenotype amongst uropathogenic *E. coli*. Structural insight into these binding activities was gained by analyzing the effect of each mutation on both mono-mannose and tri-mannose binding. Mannose binding assays were done with purified FimCH complexes as well as FimCH expressed on in tact *E. coli*.

#### **6.1.3.1 Isolated FimCH Protein**

Wild type and mutant FimCH complexes were isolated from *E. coli* and purified. The protein complexes were tested for mannose binding ability through the use of a number of different assays described below. Data is summarized in Table 8.

#### **Hemagglutination Assay**

ORN103/pUT2002 *E. coli* complemented with FimH expression constructs were induced to express FimH and other gene products in the rest of the type 1 operon. Briefly, bacteria were first grown overnight in shaking incubators at 37 °C. On the



following day, bacteria were diluted 10-fold and sub-cultured statically again overnight in the presence of 1  $\mu$ M IPTG. Hemagglutination assays with guinea pig erythrocytes were performed following published protocols (Slonim et al, 1992, *EMBO J.* 11:4747-56; Hultgren et al., 1990, *Mol Microbiol.* 4:1311-8 and Duguid et al., 1979, *J. Med. Microbiol.* 12:213). Inhibition of agglutination by a 10 mM solution of  $\alpha$ -methyl mannoside was used to demonstrate that the agglutination was dependent on mannose.

WT FimCH, FimCH S62A, and FimCH N46D gave positive results in this assay. All remaining FimCH mutations abolished the ability to agglutinate erythrocytes (*i.e.*, did not bind mannose on the erythrocyte surface).

#### Binding to Mannose-Coated Sepharose Beads

Sepharose 6B beads were coated with saturating amounts of D-mannose (Sigma) and resuspended in 0.02% Na azide, 15 mM  $\text{CaCl}_2$ , 1.25 M NaCl, 10 mM Tri-HCl, pH 7.8. Mono-mannose coated beads were washed extensively and resuspended as 50% (v/v) slurry in 20 mM MES, pH 6.8. Twenty micrograms of FimCH complexes and 100  $\mu$ l of the mono-mannose beads were used in the binding experiments. Proteins and beads were incubated together for 2 hours in a reaction volume of 200  $\mu$ l. Unbound proteins were removed and beads were washed three times with PBS. The washed beads were divided into 2 equal portions: to one half, 50  $\mu$ l of SDS-PAGE loading buffer was added for the determination of bound FimCH and 50  $\mu$ l of 1% methyl- $\alpha$ -D-mannopyranosides were added to the other half in attempt to elute bound FimCH. Elution of bound FimCH complexes were allowed to proceed for 40-60 minutes. Following elution, the supernatants were transferred to fresh tubes and proteins in the bound or eluted fractions were resolved on 15% SDS-PAGE gels. SDS-PAGE was performed following standard laboratory protocols. Gels were stained with Coomassie stain according to standard laboratory procedure to visualize the presence of FimCH.

After Coomassie staining and re-hydration, gels were dried onto cellophane sheets. FimCH bands on gels were scanned as digitized images. The quantitation of FimH-band intensity was performed with NIH Image v. 1.62. The relative amounts of FimH proteins on gels were calculated as the integrated intensity of the area surrounding the FimH band. Same area size was used to calculate the intensity of each FimH band.

WT FimCH, FimCH S62A, FimCH D140A, FimCH D140N, FimCH D140E, FimCH N46A, and FimCH N46D all bound mono-mannose coated beads to approximately the same extent. However, the relative amount of FimCH N46D, FimCH D140A, FimCH D140N, FimCH D140E, and FimCH N46A eluted by D- $\alpha$ -mannopyranoside was two- to



five-fold greater than the amount of wild type WT FimCH or FimCH S62A eluted from the same amount of beads suggesting that these mutations in FimH decreased its affinity for mono-mannose (Figures 5 A-B).

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#### Mannose Affinity Chromatography

In order to evaluate the binding affinities of FimH mutants, an HPLC-format assay was developed using a commercially available methacrylate resin (PE Biosystems) to which a tri-mannose-BSA conjugate (1-3, 1-6-D mannotriose-BSA) or a mono-mannose-BSA conjugate was coupled via epoxide chemistry. The column, which has a bed volume of 10 0.2 ml, is equilibrated with Phosphate Buffered Saline (PBS, 33.3 mM phosphate, 150 mM NaCl, pH 7.2) and run at a flow rate of 1 ml/minute. Purified FimCH complexes, containing either wild type or mutant FimH, were used in this assay. Samples were diluted to a concentration between 1 and 10 µg/ml using PBS containing 0.5 % Tween-20 (PBST). The diluted samples were filtered through a microcentrifuge filter (0.45 µm) at 13000 rpm 15 (10,000 x g) for 3 minutes at room temperature. An injected sample of proteins flowed through the column to allow interactions with the tri- or mono-mannose moieties. An injection of 50 µl of sample is followed by a 0.5-minute PBS wash. The bound FimCH is subsequently eluted with 0.1 M H<sub>3</sub>PO<sub>4</sub> + 0.15 M NaCl for 2 minutes and detected by intrinsic tryptophan fluorescence, using an excitation wavelength of 280 nm and an emission 20 wavelength of 325 nm. Finally, the column is re-equilibrated with PBS for 2.5 minutes. Affinity measurements relative to the wild type FimH can be determined for the bound FimCH complexes based upon the retention time profile.

FimCH Q133A, FimCH N135A, FimCH D140A, FimCH D140N, FimCH D140E, and FimCH N46A were retained on tri-mannose column similarly to WT FimCH. 25 However, none of the mutant FimCH protein complexes could bind to mono-mannose coated beads during this assay.

#### Solid Phase (ELISA) Binding Assay

One characteristic of the FimCH molecule is its ability to bind to mannose 30 and mannose-derivatives through the FimH portion of the molecule. The mannose solid phase binding ELISA assay was developed to measure this binding, and to assess the binding avidity differences of various mutants of FimCH for mannose derivatives. This assay exploits the mannose binding function of the FimH region of the molecule.

Immulon 4 plates were coated overnight at 4°C with 0.1 µg/well of mono- 35 mannose- or tri-mannose-BSA. On the following day, wells were blocked with 300 µl/well



of PBS+1% BSA+0.02% Sodium azide for 1 hour at 37°C followed by three washes with PBS+0.05% Tween-20 (PBST). FimCH samples were diluted in PBS+0.05% Tween-20+0.1% BSA. One hundred microliters of diluted protein samples were added into each well. Plates were incubated at 37 °C for 1 hour. After incubation with FimCH complexes, wells were washed three times with PBST. Subsequently, biotin-conjugated anti-FimC monoclonal antibody was added to each well and plates were incubated again at 37 °C for 1 hour. At the end of incubation, wells were washed as above and horseradish peroxidase-conjugated streptavidin (1:1000 dilution) (Tropix) was added. Following a 30 minute incubation at 37 °C, wells were washed again as above. ELISA reaction was developed with TMB substrate at room temperature for 10 minutes and stop reaction with 50 ul/well of 2N H<sub>2</sub>SO<sub>4</sub>. Reaction plates were read on SOFTmax at 450 nm.

Wild type FimCH was able to bind tri-mannose approximately 10 times better than mono-mannose as measured by ELISA. A two fold reduction in the relative binding of FimCH N46D to mono-mannose was also detected by ELISA however binding to tri-mannose seemed to be unaffected by the mutation. Binding to mono-mannose in the ELISA by FimCH Q133A, FimCH N135A, FimCH D140A, FimCH D140N, FimCH D140E, and FimCH N46A was undetectable with the exception of FimCH D140N, which showed very low levels of binding. Interestingly, although mutations in residue 140 greatly reduced (FimCH D140N) or abolished (FimCH D140A and FimCH D140E) mono-mannose binding in the ELISA assay, they retained their ability to bind tri-mannose, albeit at reduced levels compared to the wild type protein. (Figures 6 A-B)

#### 6.1.3.2 FimCH Protein Expressed on E. coli

*E. coli* strain PmmB66 was transfected with cDNA encoding the various FimH mutants. Because PmmB66 does not endogenously express FimH, all of the FimCH complexes on its surface will contain the FimH mutant protein. Mannose binding ability of the mutant FimCH protein when in the context of a cell surface receptor was examined by the following whole cell solid phase mannose binding assay.

Each well of an Immulon-4 plate (Dynex Technologies, Chantilly, VA) was coated with 2.5 µg/ml of mono-mannose or tri-mannose-BSA (V-labs, Covington, LA) in Carbonate Coating Buffer overnight at 4° C. The wells were aspirated and then blocked with PBS + 1% BSA (300 ml/well) by incubation at 37° C for 1 hour. Plates were then washed three times with PBS + 0.1% Tween + 0.1% BSA. The *E. coli* expressing either wild type or mutant FimCH ( $8.0 \times 10^7$  CFU/ml) were added to each well and incubated at 37°C for 1 hour, and then washed extensively. Bound bacteria were detected with a 1:400



dilution of a polyclonal anti-*E. coli* (all antigens)-peroxidase conjugated antibody (BioDesign, Inc., Kennebunk, ME; catalog no. B65004R). After washing three times with PBS + 0.1% Tween + 0.1% BSA, the TMB substrate (100 ml/well) was added and incubated at ambient temperature for optimal time before stopping with 2N H<sub>2</sub>SO<sub>4</sub>. OD<sub>450</sub> readings were taken to quantify the amount of bacteria bound to the mannose.

FimCH N46D could bind tri-mannose at near wild type levels but had a decrease in its ability to bind mono-mannose (Figure 7E). FimCH S62A could bind mono- and tri-mannose equally well, but at a level that was somewhat decreased from wild type ability (Figure 7H). No significant binding could be detected for FimCH N46A, FimCH D140E, and FimCH Q133K (Figures 7D, 7F, and 7G) on either mono- or tri-mannose. These results are similar to those obtained when testing mannose-binding ability of isolates mutant FimCH proteins (see Section 6.1.3.1).

As a control, plates were coated with the polyclonal anti-*E. coli* antibody and then exposed to *E. coli* expressing the different FimCH mutant proteins. Figure 7I shows that the polyclonal antibody can bind to each of the mutant-expressing *E. coli* equally well. This indicates that any differences in the amount of *E. coli* detected in Figures 7A-H reflect a true difference in mannose binding instead of a technical difficulty with the detection method.

#### 6.1.4 Adherence and Invasion Assays

AAEC185/pUT2002 transformed with FimH expression plasmids were used to assay FimH-mediated bacterial adherence and invasion into the human bladder cell line 5637 (ATCC # HTB-9). Bacteria were cultured as described above for type 1 pili expression. Adherence and invasion assays were performed following published protocols with a minor modification (Elsinghorst & Weitz, 1994, *Infect Immun.* 62:3463-71; Martinez *et al.*, 2000, *EMBO J.* 2000 19:2803-12). Instead of a two-hour infection step, bacteria were incubated for one hour to allow for binding and entry into bladder cells.

WT FimCH, FimCH S62A, and FimCH N46D could adhere and invade the bladder cells (although FimCH N46D had a 2-fold decrease in ability when compared to WT FimCH). All of the remaining mutant FimCH proteins, however, had no ability to adhere or to bind bladder cells (Figure 8A). However, all of those *E. coli* expressing a FimCH complex competent to adhere to 5637 cells, could also invade (Figure 8B).

*E. coli* expressing FimCH proteins were also tested for the ability to bind human bladder tissue sections. AAEC185/pUT2002 transformed with FimH expression plasmids were used to assay FimH-mediated bacterial adherence to tissue sections. Bacteria



were cultured as described above for the optimal expression of type 1 pili. *In situ* binding to human bladder tissues was performed similarly to previously described protocol with minor modifications (Striker, 1995, *Adv Exp Med Biol.* 385:141-2; Falk *et al.*, 1993, *Proc. Natl. Acad. Sci. USA*, 90:2035-2039). Briefly, overnight cultures were diluted to the same  
5 concentration (OD<sub>600</sub> 1) and 1 ml of each diluted bacteria was labeled with fluorescein isothiocyanate (FITC) as described (Falk *et al.*, 1993, *Proc. Natl. Acad. Sci. USA*, 90:2035-2039). Labeled bacteria were resuspended in 1 ml blocking buffer (PBS+0.25% BSA+0.05% Tween-20). Non-diseased human bladder sections were obtained from the  
10 surgical pathology and autopsy files of the Department of Pathology at Washington University and deparaffinized following published protocol Falk *et al.*, 1993, *Proc. Natl. Acad. Sci. USA*, 90:2035-2039. Human bladder tissues on microscope slides were incubated with 100 ul of freshly FITC-labeled bacteria for 2 hours at room temperature in a humidified chamber. Following bacterial binding, slides were washed extensively with PBS, and fixed  
15 for 5 minutes with 2.5% glutaraldehyde in PBS. After fixation, slides were counterstained with 1 µg/ml Hoechst stain for 5 minutes. Upon mounting with cover slips, slides were dried overnight at room temperature in the dark. Visualization of bound bacteria was performed on an Olympus BX60 microscope system.

Both WT FimCH and FimCH S62A mediated a high level of tissue binding in a mannose-inhibitable fashion (Figures 9A-D). Bacteria were seen binding to the luminal  
20 surfaces of the bladder sections as well as the sub-layers of the bladder epithelium. FimCH N46D could adhere and invade the bladder cells albeit it had a 2-fold decrease in ability when compared to WT FimCH (Figures 9E-F). Binding mediated by FimCH N46D was inhibited by soluble mannose (Figure 9G). None of the other mutants tested showed  
25 significant binding or invasion. (Figures 9H-K). (Data is summarized in Table 8).

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Table 8

FimH protein	Pilus Localization	HA	Mannose Binding								Bladder Cell Adherence	Invasion
			Affinity Chromatography		Beads		ELISA		ELISA			
			Tri-mannose	Mono-mannose	Tri-mannose	Mono-mannose	(with purified FimCH)	(with FimCH on E. coli)	Tri-mannose	Mono-mannose		
WT	+	+	+	+	+	+	+	+	+	+	+	+
I13A	+	nd	nd	nd	nd	+	+	+	+	nd	nd	nd
S62A	+	+	nd	nd	nd	+	+	nd	nd	+	+(7)	+
N46D	+	+	nd	nd	nd	nd	+(1)	+	+(5)	+	+/-	+
N46A	+	-	nd	nd	nd	nd	+(1)	nd	-	-	-	-
Y48A	+	nd	nd	nd	nd	nd	nd	+	+	nd	nd	nd
I52A	+	nd	nd	nd	nd	nd	nd	+	+/- (6)	nd	nd	nd
D54A	+	-	-	-	-	-	-	-	-	nd	nd	-
D54N	+	-	-	-	-	-	-	-	-	nd	nd	-
Q133K	+	-	-	-	-	-	-	-	-	-	-	-
Q133A	+	-	+	nd	+	+	+/- (2)	nd	-	nd	nd	-
Q133N	+	-	-	-	-	-	-	-	-	nd	nd	-
Q133E	+	nd	nd	nd	nd	nd	nd	+	+/- (6)	nd	nd	nd
Q133H	+	nd	nd	nd	nd	nd	nd	-	-	nd	nd	nd
Q133R	+	nd	nd	nd	nd	nd	nd	-	-	nd	nd	nd
N135A	+	-	+	nd	+	+	+/- (2)	nd	-	nd	nd	-
N135D	+	-	-	-	-	-	-	-	-	nd	nd	-
Y137A	+	nd	nd	nd	nd	nd	nd	+	+/- (6)	nd	nd	nd
D140E	+	-	+	nd	nd	nd	+(1)	+(4)	-	-	-	-
D140A	+	-	+	nd	nd	nd	+(1)	+(4)	-	nd	nd	-
D140N	+	-	+	nd	nd	nd	+(1)	+(4)	+/-	nd	nd	-

nd indicates not determined

- (1) WT and mutant protein bind to mono-mannose beads in equal amounts; mutant protein elutes with  $\alpha$ -D-mannopyranoside 2-5 fold more easily
- (2) mutant protein binds mono-mannose beads less well than WT protein and elutes with  $\alpha$ -D-mannopyranoside 4-5 fold more easily
- (3) WT protein binds tri-mannose 10 fold better than mono-mannose as assayed by ELISA
- (4) mutant proteins bind tri-mannose at reduced levels when compared to WT protein (D140N binds tri-mannose as well as WT binds mono-mannose)
- (5) WT protein binds 2 fold better than mutant protein
- (6) mutant protein binds higher concentration of mono-mannose at 30%-50% WT levels
- (7) mutant protein binds mono- and tri-mannose equally well but decreased from WT levels



### 6.1.5 Naturally Occurring FimH Mutant

All of the mutations in the mono-mannose binding pocket completely abolished binding to bladder epithelium except for the N46D mutation. The N46D mutation reduced binding to bladder cells by about 50%. It retained the ability to bind tri-mannose with the same relative affinity as wild type FimH but had approximately a 50% reduced affinity for mono-mannose. Thus, mono-mannose but not tri-mannose binding appears to be strictly correlated with the physiologically relevant function of FimH in binding bladder epithelium. Since the amide oxygen that binds O6 is left intact in the N46D mutant, the 50% reduction in mono-mannose and bladder binding is presumably a result of the inability to stabilize the pocket to the same degree as the wild type. Thus, even the slightest change in the mannose binding pocket, in an atom that does not directly bind mannose, still significantly reduces binding, emphasizing why the pocket is invariant amongst 200 uropathogenic isolates (see, e.g., Figure 3).

Enterohemorrhagic *E. coli* (EHEC) are the cause of hemolytic uremic syndrome which results in acute kidney failure (Noel *et al.*, 1997, *Dig. Dis.* 15:67-91). This syndrome is thought to be the effect of the Shiga toxin, that enters the blood stream and locates to the kidney due to its receptor binding specificity (Kiyokawa *et al.*, 1998, *J. Infect. Dis.* 178:178-184; Cooling *et al.*, 1998, *Infect. Immun.* 66:4355-4366). Although EHEC possess the type 1 pilus gene cluster, there is a lack of an association of EHEC strains with urinary tract infections. Interestingly, an inspection of the FimH gene sequences from three different enterohemorrhagic strains revealed that the binding pocket residue Asn135 was changed to a lysine (this sequence is depicted in Figure 3 as EC189). A lysine at this position would be predicted to exclude mannose from the binding pocket. A dysfunctional mono-mannose binding pocket would render EHEC unable to colonize the bladder and establish an infection. This may represent a natural selection for a less virulent phenotype since colonization of the urinary tract would lead to a direct delivery of the toxin to the kidney causing drastic and rapid consequences to the host.

## 6.2 EXAMPLE 2: Production of Antibodies

### 6.2.1 Polyclonal Antibodies

The immunogenicity of purified FimCH variant proteins were assessed by measuring immunoglobulin G (IgG) titer to FimH T3. FimH T3 is a histidine-tagged fusion protein composed of the first 165 amino acids of the mature (279 amino acids) FimH protein.

C3H/HeJ mice were immunized on day 0 (primary immunization) and booster immunized during week 4 with one of the 7 purified antigens: wild type FimCH (from strain J96), wild type FimCH (vaccine composition), FimCH D140E, FimCH N46D,



FimCH Q133K, FimCH Q133E, and FimCH Q133H. Injections were at doses of 4.0, 1.6, 0.64, and 0.26 µg in MF59 adjuvant (Chiron, Emeryville, CA).

Samples from individual mice treated identically were pooled for serological analysis and diluted 1:100 before serial dilution. Antibody responses were assessed by an ELISA with purified FimH T3 as the capture antigens. The purity of the protein preparations of the capture antigen was 95% pure for FimH T3. In all cases the protein preparations were free of any lipopolysaccharide contaminants. Data for immune responses of such mice to the various FimH adhesins is in Figures 10A-C.

Mice vaccinated with FimCH N46D and FimCH D140E showed comparable response to FimCH T3 by ELISA both at 3 weeks (pre-boost) and at 8 weeks (4 weeks post boost) at all doses when compared to wild type FimCH (Figure 10A and 10B).

Interestingly, mice vaccinated with FimCH Q133K protein induced titers to FimH T3 at 3 weeks (pre-boost) that were approximately 20 fold lower than titers to wild type FimH at all doses. However, titers from the FimCH Q133K immunized mice did increase following the boost at 4 weeks and were now comparable to the wild type protein (Figure 10C). This was true at all doses.

### 6.2.2 Monoclonal Antibodies

Monoclonal antibodies (MAB) were made directed against purified WT FimCH or FimCH Q133K protein using standard techniques well known in the art. Various proteins were used at a 1 µg/ml concentration as capture antigens in an ELISA assay to determine the epitope of each monoclonal antibody clone. Capture antigens included FimC alone (Table , row 1), wild type and mutant FimCH complexes (Table 9, rows 2-8), and truncated FimH proteins (rows 9-11; T3 is a histidine tagged N-terminal lectin binding domain of FimH from amino acid residues 1-184; T2B is the N-terminal lectin binding domain of FimH from amino acid residues 1-178). FimH specific clones were identified based on positive reactivity with the FimCH or FimCH Q133K complex and a negative reactivity with FimC alone by ELISA (Table 9, compare rows 1-3). Clones 1A7, 1C10, 3E11, and 1F2 bind an epitope on FimH while clones 2B2 and 4G3 bind an epitope on FimC. Interestingly, not all MAB clones that bind to FimH do so equally well. For example, clone 1A7 bound FimCH Q133K better than WT FimCH and did not bind FimCH N135D and FimCH D54A at all (Table 9, rows 2-5) while clone 1C10 bound all FimH-containing complexes equally well (Table 9, rows 2-8).



Table 9: Binding specificity of monoclonal antibodies

	1A7	1C10	3E11	1F2	4G3	2B2	positive control
1 - FimC	0.038	0.037	0.039	0.04	0.553	0.697	0.982
2 - FimCH WT	0.328	0.624	0.098	0.845	0.793	1.04	1.1
3 - FimCH Q133K	0.504	0.710	0.318	0.555	0.616	0.900	1.1
4 - FimCH N135D	0.04	0.668	0.038	0.643	0.694	0.951	1.1
5 - FimCH D54A	0.055	0.600	0.042	0.735	0.752	1.02	1.17
6 - FimCH Q133A	0.476	0.734	0.370	0.761	0.734	0.988	1.1
7 - FimCH Q133N	0.351	0.757	0.160	0.700	0.705	0.948	1.1
8 - FimCH D140A	0.093	0.710	0.05	0.828	0.750	1.01	1.15
9 - FimH T3	0.616	0.995	0.204	0.104	0.469	0.047	1.1
10 - FimH T2B Q133K	0.283	1.0	0.180	0.187	0.621	0.046	1.1
11 - FimH T2B WT	0.334	1.04	0.092	0.092	0.116	0.045	1.2

Further information regarding the type of epitope recognized by each MAB clone was obtained by western blot analysis as well as by ELISA under urea-denaturing conditions. Western blotting was carried out according standard laboratory protocols also. Briefly, proteins in SDS-PAGE gels were transferred to PVDF membranes (Schleicher & Schuel) and blocked for one hour in blocking buffer consisting of TBST (500 mM NaCl, 0.05% Tween-20, 20 mM Tri-HCL, pH 7.5)/5% nonfat dry milk/3% bovine serum albumin (BSA). Blots were washed briefly in TBST and incubated with anti-FimC/FimH mouse antiserum diluted 1000-fold in blocking buffer for one hour. Following primary antiserum incubation, blots were washed three times for 5 min each with TBST and incubated for another hour with alkaline phosphatase (AP)-conjugated goat  $\alpha$ -mouse IgG (whole molecule) secondary antibody (Sigma) diluted 2000-fold in blocking buffer. Subsequently, blots were washed four times for 5 min each with TBST and once with developer buffer (100 mM NaCl, 5 mM MgCl, 100 mM Tri-HCl, pH 9.5) and then developed with 0.04% NBT+0.02% BCIP (diluted in developer buffer).

The results are summarized in Table 10. Briefly, 1A7 and 1C10 cannot recognize FimCH Q133K protein when the protein is denatured indicating that a conformational epitope is recognized. Alternatively, 1F2 can recognize denatured protein indicating that a linear epitope is recognized.



Table 10: Characterization of MAB against FimCH Q133K

MAB clone	epitope	western blot	ELISA with urea-denatured protein
1A7	bind FimH	no	no
1C10	bind FimH	weak	no
3E11	bind FimH	nd	nd
2B2	bind FimC	nd	nd
1C8	bind FimC	strong	nd
1F2	bind FimH	strong	yes

nd indicates not determined

### 6.3 EXAMPLE 3: Inhibitory Properties of Polyclonal Antibodies

#### 6.3.1 *in vitro*

Functional inhibitory properties of polyclonal antibodies were measured by the ability to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to guinea pig erythrocytes in a hemagglutination assay and by the ability to inhibit *E. coli* binding to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to transformed human bladder J82 cell line.

#### Hemagglutination Assay

The bacteria were directly labeled with fluorescein isothiocyanate (FITC) and incubated with the antibody to be assayed for 30 minutes at 37°C. The bacteria/antibody mixture was then added to the erythrocytes and allowed to incubate. After multiple washes, mean channel fluorescence was used as an indicator of the amount of FITC-labeled bacteria remaining (and thereby is an indication of the strength of the interaction between the FimCH complex on the *E. coli* and mannose). Lysis II software (Becton Dickinson Immunocytometry Systems) was used for analysis of data.

Figure 11 shows the results from the hemagglutination assay. Increasing dilutions of polyclonal antibodies were used in a set of parallel experiments. Preincubation with polyclonal antibodies raised against FimCH Q133 E, FimCH Q133H, FimCH Q133R, FimCH N135D, and WT FimCH inhibited bacteria binding to the erythrocytes very strongly. Polyclonal antibodies raised against FimCH Q133E and FimCH Q133H were inhibitory at greater dilutions than those used for polyclonal antibodies raised against wild type protein (8-32 times more diluted). Control antiserum from animals that were either not immunized or immunized with MF59 adjuvant alone showed no inhibition.



### Inhibition of Binding to Bladder Cells

Functional inhibitory properties of antibodies were measured by the ability to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to transformed human bladder J82 cell line (American Type Culture Collection Accession Number HTB1). The bacteria were directly labeled with fluorescein isothiocyanate (FITC) and incubated with the antibody to be assayed for 30 minutes at 37°C. The bacteria/antibody mixture was then added to 1x10<sup>6</sup> bladder cells at a ratio of 250 bacteria/cell. After multiple washes, samples were assayed by flow cytometry (FACStar PLUS; Becton Dickinson, San Jose, CA) as described in Langermann *et al.* (1997, *Science* 276:607-11; which is hereby incorporated by reference in its entirety). Mean channel fluorescence was used as an indicator of FITC-labeled bacteria bound to the J82 bladder cells. Lysis II software (Becton Dickinson Immunocytometry Systems) was used for analysis of data.

The above functional inhibitory assay was performed using the mutant FimH proteins of the invention. Inhibitory assays were run with the 8 week antisera (4 weeks post boost) from mice vaccinated with FimCH N46D and FimCH D140E and the antisera showed comparable inhibitory titers to the anti-FimH wild type antisera. (Figure 12A and 12B).

Although the absolute titers were low, antibodies to FimCH Q133K had a better *in vitro* functional inhibitory activity when compared to wild type FimH antibodies (Figure 12C). This trend toward superior inhibitory function continued past the 4 week boost. Antisera from mice receiving the 4.0, 1.6, and 0.64 doses of the FimCH Q133K protein was still 100% inhibitory at a 1:1600 dilution. Antisera from mice receiving the 0.26 dose of the mutant protein was still 75% inhibitory at the 1:1600 dilution. This is contrasted with the endpoint inhibitory titer of 1:400-1:800 dilution seen at the highest dose (4.0 µg) for wild type FimCH protein.

For wild type FimCH and FimCH Q133K, an additional boost at week 18 was given. Inhibitory assays were done with antisera from week 16 and week 20. At week 16 (before the second boost), anti-wild type FimCH antibodies did not inhibit bacteria binding to the bladder cells well (Figure 12D). This is contrasted with anti-FimCH Q133K antibodies. At higher concentrations of antibodies (*i.e.* 1:50, 1:100, and 1:200 dilutions), the pre-second boost anti-FimCH Q133K still retain inhibitory ability (Figure 12E). At 20 weeks (2 weeks post second boost), the anti-wild type FimCH antibody does regain some inhibitory ability but it is not as dramatic as the anti-FimCH Q133K antibody.

Polyclonal antibodies to WT FimCH can inhibit bacteria binding to uroepithelial cells from diabetic women. Uroepithelial cells were isolated from the urine of



diabetic women. FITC-labeled *E. coli* strain NU14 (expressing WT FimCH) was incubated with polyclonal antibodies to FimC, FimH or FimCH. This decreased bacterial binding to the uroepithelial cells by 65% (data not shown).

### 6.3.2 *in vivo*

Mice were passively immunized with polyclonal antibodies generated with either WT FimCH or mutant protein (FimCH N135D or FimCH Q133R). Mice were administered 1 mg of polyclonal antibody 4 hours prior to a large bolus challenge live uropathogenic *E. coli*. Type 1 piliated *E. coli* strain (NU14) bacteria were collected, washed and re-suspended in phosphate buffered saline (PBS) and cell concentration adjusted to OD = 1.8 (at 600 nm). This bacterial cell suspension was then diluted 1:10 in PBS and used as inoculum. Mice were anaesthetized and then inoculated intraurethrally with 50 µl of *E. coli* suspension containing about  $3 \times 10^7$  CFU (colony forming units). CFU determination was done by plating the bacterial suspension on TCA plates and examining cell viability. Two days post-inoculation, the mice were sacrificed and bladders were removed and collected into 500 µl PBS supplemented with 1% mannose. The number of CFUs per bladder was determined by grinding the bladders with a tissue tearer and then plating the suspension on TSA plates after dilution. The mean number of colony forming units per bladder was determined and data was transformed to log CFU/bladder. A decrease in the number of CFUs indicates that the passive immunization had a protective ability. Polyclonal antibodies to both mutant proteins were more protective than those raised against wild type protein (Figure 13). The decrease in CFUs per bladder obtained by administration of polyclonal antibodies raised against mutant FimCH was significant when compared to CFUs per bladder obtained when no antibody was administered as indicated by a T-test (see Table 11).

Table 11: T-test Results

antigen polyclonal antibody raised against	MF 59 alone	no injection
FimCH	0.190	0.581
FimCH N135D	0.00003	0.0043
FimCH Q133R	0.0004	0.080



## 6.4 EXAMPLE 4: Inhibitory Properties of Monoclonal Antibodies

### 6.4.1 in vitro

Functional inhibitory properties of antibodies were measured by the ability to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to guinea pig erythrocytes in a hemagglutination assay and by the ability to inhibit *E. coli* binding to an ELISA plate when tri-mannose was the capture antigen. Fab fragments were also assayed for inhibitory activity.

#### Hemagglutination Assay

The bacteria were directly labeled with fluorescein isothiocyanate (FITC) and incubated with the antibody to be assayed for 30 minutes at 37°C. The bacteria/antibody mixture was then added to the erythrocytes and allowed to incubate. After multiple washes, mean channel fluorescence was used as an indicator of the amount of FITC-labeled bacteria remaining (and thereby is an indication of the strength of the interaction between the FimCH complex on the *E. coli* and mannose). Lysis II software (Becton Dickinson Immunocytometry Systems) was used for analysis of data.

Figure 14 shows the results from the hemagglutination assay. Increasing dilutions of MAB clone were used in a set of parallel experiments. Preincubation with clone 1A7 inhibited bacteria binding to the erythrocytes very strongly. Clones 1C10 and 3E11 also inhibited bacteria binding when the MABs were supplied in larger quantities. Clones 1F2, 2B2, and 1C8 did not show an inhibitory activity. Figure 15A shows the results of various concentrations of clone 1A7 used in the hemagglutination assay. Figure 15B shows various controls that indicate that this inhibitory activity was due to preincubation with MAB clone 1A7. Guinea pig red blood cells alone do not fluoresce. *E. coli* Nu14 bind to guinea pig red blood cells in the absence of antibody pre-incubation. Pre-incubation of *E. coli* with pre-immune serum does not inhibit binding to guinea pig red blood cells. As expected, pre-incubation with antibodies raised against T3 (a histidine tagged N-terminal lectin binding domain of FimH from amino acid residues 1-184) does inhibit *E. coli* binding to guinea pig red blood cells.

#### ELISA Binding Assay

Immulon 4 plates were coated overnight at 4 °C with 0.1 µg/well of tri-mannose-BSA. On the following day, wells were blocked with 300 ul/well of PBS+1% BSA+0.02% Sodium azide for 1 hour at 37 °C followed by three washes with PBS+0.05% Tween-20 (PBST). *E. coli* that had been pre-incubated with the antibody to be assayed (for 30 minutes at 37°C) was added to the tri-mannose coated well. After incubation, the wells were washed extensively. Optical density at 450 nm (OD<sub>450</sub>) was recorded and used as an indicator



of the amount of bacteria attached to the tri-mannose.

Figure 16 shows the results from the ELISA assay. Pre-incubation of bacteria with either MAB clone 1A7 or 1C10 did inhibit binding to tri-mannose as evidenced by the decrease in OD<sub>450</sub> with increasing MAB antibody used. MAB clone 1C8 (which recognizes an epitope on FimC) did not demonstrate any inhibitory effect at any amount of MAB used and thus mimicked the negative control data.

#### Characterization of Fab Fragments

Fab fragments were generated for MAB clones 1A7, 1C10, and 1F2. Fabs were purified before use as potential inhibitors of FimCH-mannose binding in a hemagglutination assay. The assay was done as previously, with results shown in Figure 17. Fab fragments of clone 1A7 inhibited bacteria binding as well as intact MAB clone 1A7. This suggests that clone 1A7 inhibits FimCH binding through a steric hindrance of binding versus agglutination. However, Fab fragments of clone 1C10 displayed a drastic decrease in inhibitory ability when compared with its intact MAB counterpart. This suggests that agglutinating activity is an important part of clone 1C10 MAB's inhibitory activity.

#### 6.4.2 in vivo

Passive immunization protection studies were done with MAB clones 1A7, 1C10, and 1F12. One mg of purified MAB was administered by IP injection to a C3H/HeJ mouse. Four hours after MAB administration, the mouse was challenged intraurethrally with  $8.2 \times 10^7$  CFU of uropathogenic *E. coli* NU14. After 48 hours, the animal was sacrificed and the bladder was harvested to determine the resulting CFU per bladder.

Figure 18 shows the results of the passive immunization experiment. MAB clone 1C10 provided significant protection (1.4 log reduction in CFU) against *E. coli* infection. However, neither MAB clone 1A7 or 1F2 showed the ability to protect against the large bolus challenge. The decrease in CFUs per bladder obtained by 1C10 administration was significant when compared to CFUs per bladder obtained when no MAB was administered as indicated by a T-test (see Table 12).

Table 12: T-test Results

MAB clone	no injection
1A7	0.271
1C10	0.002
1F2	0.024



### 6.5 EXAMPLE 5: Use of Mutant Proteins as Vaccines

The purpose of these studies is to examine the efficacy of FimCH mutant to induce a protective immune response in primates.

#### 6.5.1 Monkey Vaccination

A recombinant FimC and a mutant FimH complex is purified to over 99% purity from the periplasm of *E. coli* K12 strain 600 as described in Jones *et al.* (1993, *Proc. Natl. Acad. Sci. USA* 90:8397-401).

Bacteria is cultivated in LB agar. Expression of type 1 pili is induced by two 48 hour passages in static brain-heart infusion broth (Difco Labs, Detroit) culture at 37°C. Before infection, expression of type 1 pili is quantitated by titration of bacterial suspension and mixing of equal volumes of 3% yeast cells and bacteria in microtiter cells to assay agglutination titers (titers equal to or over 30-60 indicate type 1 pili expression). After bacterial challenge in the monkeys, urine samples from days 2, 4, 7 and 12 after challenge are counted by streaking 100 L of serial 10 step dilution onto cystine-lactose-electrolyte deficient agar plates by means of sterile plastic disposable loops. After incubation overnight at 37°C, *E. coli* colonies are counted to establish the number of CFU/ml in the urine. A urine specimen is considered positive when it contains at least 100 CFU/ml. To establish that inoculating strain was recovered in urine, urinary bacteria are biochemically analyzed on prepared microplates for rapid typing of coli form bacteria using PhenePlate systems.

The surfactant stabilized emulsion adjuvant MF59 is used to emulsify the mutant FimCH complex and for adjuvant administration. Cynomolgus monkeys receive either 100 µg of mutant FimCH in MF59 adjuvant at a 1:1 ratio, or MF59 plus diluent at weeks 0, 4, and 48. Each 1 ml injection is administered intramuscularly in the thigh (legs are alternated for each injection). Serum samples are collected once a month after vaccination for assessment of immune responses.

Vaginal wash and serum samples are also collected before and after the last boost (weeks 47 and 50). The vaginal wash samples are diluted 1:2 in 0.5% bovine serum albumin, 0.5% milk and 0.2% azide before analysis. Antibody levels are recorded as actual OD at 405 nm (values <2x background were considered negative).

In addition, functional assays are performed with the serum and vaginal washes to demonstrate the efficacy of the vaccine to induce an anti-FimH immunoglobulin response.

With respect to the serum samples, type 1 pilated NU14 *E. coli* are directly labeled with fluorescein isothiocyanate and incubated with 10<sup>6</sup> J82 bladder cells at a ratio of



250 bacteria/cell in the presence of preimmune or immunized serum and incubated for 30 minutes at 37°C. After multiple washes, samples are assayed by flow cytometry, and percent inhibition is determined relative to preimmune samples from each monkey.

5 Vaginal washes are also tested to determine if the titer of antibodies in the washes of vaccinated subjects are sufficient to inhibit *E. coli* binding to trimannose. Briefly, 2.5 µg/ml of trimannose-bovine serum albumin is coated on Immulon-4 plates (Dynex Technologies, Chantilly, VA). Type 1 piliated NU14 bacteria ( $8.0 \times 10^7$  CFU/ml) is added to each well, incubated at 37°C for one hour, washed extensively and bound bacteria are detected with 1:400 dilution of anti-*E. coli* horseradish peroxidase conjugated antibody (BioDesign, Kennebunk, ME). Percent inhibition is assessed as a ratio, where % inhibition = [(full signal values - sample value)/full signal value] x 100.

10 All test monkeys are infected 18 days after the final immunization with *E. coli*. Bladder infection is induced by inoculation of bacterial suspension (1 ml,  $10^8$  CFU/ml) via urethral catheter. Urine samples are obtained on days 2, 4, 7, 12 and 14 after challenge to determine the number of bacteria per milliliter of urine, as a measure of infection. Urine samples are also tested for leukocytes as an indicator of inflammation.

15 Normal flora is also tested to determine whether systemic vaccination with the mutant FimCH adhesin polypeptide affects the normal intestinal flora. *E. coli* recovered from fecal suspensions from each monkey is tested in the PhP assay. All monkeys in both vaccine groups showed normal coliform bacterial growth.

### 6.5.2 Human Vaccination

20 Recombinant highly purified mutant FimCH is formulated in the squalene-based adjuvant MF59C.1 to examine safety and immunogenicity in a randomized, controlled, double blind Phase I clinical trial in healthy adult women who are seronegative for anti-FimH antibodies.

#### Methods

30 The soluble 52 kDa recombinant protein complex of FimC and mutant FimH, FimCH, is recovered from lysed bacteria using a three step chromatographic process. The bulk product is sterile filtered and vialled in a citrate buffer. Shortly before injection into a subject, the FimCH composition is mixed with a squalene-based emulsion adjuvant known as MF59C.1 (Chiron Corp., CA).

35 *In vitro* binding to human tissues, purified receptors or receptor homologues is often used to elucidate the roles in virulence of many different adhesins, including pilus-associated adhesins. Similarly, assaying for the ability of such antibodies to block



attachment of bacteria to cells or specific receptors can assess the functionality of antibodies to adhesins. This allows for rapid *in vitro* assessment of serological cross-reactivity between antibodies raised to a single adhesin, such as FimCH purified from one strain of *E. coli*, against a wide range of *E. coli* clinical isolates expressing highly homologous, yet phenotypically distinct FimH adhesins.

The ability of the anti-FimH adhesin antibodies to block bacterial binding to bladder epithelial cells is investigated *in vitro* using a flow cytometric method originally developed for evaluating Rickettsia-cell attachment (Li and Walker, 1992, Infect Immun. 60:2030-5, which is incorporated herein in its entirety).

The bacterial binding inhibition assay is run as follows. Type 1-piliated *E. coli* (cystitis, pyelonephritis, gut etc.) isolates are directly labeled with FITC and incubated with  $2 \times 10^6$  J82 bladder cells, at a ratio of 250 bacteria/cell, in the presence of pre-immune or hyper-immune serum (murine, rabbit, primate or human antisera) and allowed to mix with the bacteria for 30 minutes at 37°C. Antisera are added at dilutions typically ranging from 1:50 to 1:6400 (two-fold serial dilutions). After multiple washes, samples are assayed by flow cytometry in a FACStar PLUS (Becton Dickinson) according to previously published methods (Langermann *et al.*, 1997, *Science*, 276:607-11). Mean channel fluorescence is used as an indicator of FITC-labeled bacteria bound to J82 bladder cells.

Endpoint inhibitory titers are defined as the titer, after serial two fold dilutions, at which the MCF value (representing bacteria bound to cells) is less than or equal to 50% of the MCF value for the control samples (where control is bacteria incubated with pre-immune serum). To confirm binding and inhibition, J82 bladder cells can be sorted from the flow cytometric adherence assay described and analyzed by fluorescent microscopy and the number of fluorescent bacteria attached to 40 bladder cells visually quantitated.

This assay can be run with vaginal wash samples as long as the samples are collected by straight lavage ("PBS washes"). For vaginal wash samples, inhibitory titer ratios are measured for all samples at a 1:2 dilution. Inhibition cannot be run with vaginal antibody samples collected by the cel-wec method, as this method relies upon a detergent-based extraction buffer which interferes with the binding assay.

Functional inhibitory antibodies to FimCH are also evaluated in an assay called the *E. coli* trimannose-binding assay. Briefly, Immulon-4 plates (Dynex Technologies, Inc., Chantilly, VA) are coated with 2.5 µg/ml (100 µl/well) of tri-mannose-BSA (V-Labs, Covington, LA). Type 1-piliated NU14 ( $8.0 \times 10^7$  CFU/ml) are added to each well, incubated at 37°C for 1 hour and after extensive washing, bound bacteria are detected with a 1:400 dilution of an anti-*E. coli*-HRP conjugated antibody (BioDesign, Kennebunk, ME). OD<sub>450</sub> readings of these samples establish the full signal values (FSV) for binding to trimannose



(approximately 2.0). Additional samples are run in the presence of 1:50 dilutions of serum to assess inhibition, where percent inhibition equals the FSV - the sample value/FSV x 100. All samples are run in triplicate.

Antibody sampling of vaginal secretions from primates was performed with a sterile cotton swab. The swab was then suspended in 1 ml of PBS, yielding the solution to test for antibodies. The samples were centrifuged at 2,000 X g for 10 minutes at 4°C. The supernatant was treated with Nonidet P-40, aliquoted and stored at -70°C. Antibody sampling of cervical secretions from humans was performed using an absorbent sponge called a Cel-Wec. Cervical secretions (Immunoglobulin) were eluted from sponges "Weck-Cel Spears" with elution buffer: 1 x PBS, 0.5% IGEPAL® (nonionic detergent), Protease inhibitors (1 mg/ml Aprotinin, 1 mM Leupeptin, Bestatin). Antibody sampling of urine samples was done on straight, undiluted urine samples from "clean catch" specimens.

#### Quantitation of Human IgG in Serum/Urine/Cervical Secretion Samples

##### ELISA Procedure

96 well ELISA plates are coated with capture antibody:

mouse anti human IgG (1 µg/ml CO3 buffer)

Standard\*: Human IgG whole molecule (1000 ng-977 pg/ml)

Samples: Human urine or cervical secretions in PBS (diluted two fold 1:2 to 1:64)

Secondary: Biotin labeled goat F(ab'2) anti-human IgG

Tertiary: streptavidin Horse Radish Peroxidase

Substrate: TMB

Plates are read at 450nm and quantity determined by SOFTmax software

\* to generate a standard curve this is run along with the urine, cervical secretion samples

In order to determine IgG quantity, each urine and cervical secretion sample is run in duplicate at six different dilutions (for all individuals tested). The quantity for each dilution is automatically calculated by SOFTmax using a 4 parameter standard curve (range 1000 ng-977 pg/ml). Only the quantities derived from OD values that fall within the linear range of the standard curve are used to determine the amount of IgG in a serum sample. These quantities are averaged to determine amount of IgG in a sample.

##### Clinical Procedures

Four cohorts of 12 subjects are randomized at a ratio of 3:1 (i.e., four groups where nine subjects receive the vaccine and 3 subjects receive the adjuvant alone) and, in a sequential fashion, given intramuscular doses of vaccine or control. Mutant FimCH is prepared for injection into a subject immediately prior to the injection, i.e., mixed with diluent and adjuvant. Doses of either 1, 5, 25 or 123 µg of mutant FimCH in 0.5 ml of MF59C.1, or



the control (MF59C.1 alone) are injected slowly, *i.e.*, 20 to 30 seconds, into the deltoid muscle of the upper arm of the subjects at day 0, followed by a booster dose at about 28 days followed by a second booster dose at about 180 days.

To test if the mutant FimCH vaccine is immunogenic in the human subjects, evidence of a clear dose response is looked for. Serum, urine, and vaginal secretions of vaccine recipients is used in Western blot and ELISA assays to determine levels of anti-mutant FimH antibodies. Also, immune serum from vaccine recipients is assayed for inhibitory activity by addition to uropathogenic *E. coli* before exposure to J82 human uroepithelial cell line (bladder cells) *in vitro*. Inhibition of binding of *E. coli* to J82 cells indicates the presence of inhibitory antibodies.

## 6.6 EXAMPLE 6: Preparation Of Co-Crystals Of FimCH and $\alpha$ -D-Mannopyranoside

The subsections below describe the production of the FimCH complex and the preparation and characterization of diffraction quality co-crystals of FimCH with  $\alpha$ -D-mannopyranoside.

### 6.6.1 Production and Purification of FimCH

Plasmid pHACW18 was constructed by cloning *fimH* into the EcoR I and BamH I sites of pUC18 (Norlander *et al.*, 1983 *Gene* 26:101-6). Briefly, the *fimH* gene was amplified from pHJ20 (Jones *et al.*, 1995 *Proc Natl Acad Sci USA* 92:2081-5) by polymerase chain reaction (PCR) using Vent Polymerase (New England Biolabs). The resulting *fimH* gene was confirmed by sequencing. Plasmid pHJ9205 contained the *fimC* open reading frame driven by the inducible arabinose promoter and was used for the co-expression of FimH proteins. The plasmid pUT2002 having a *fimH* deleted type 1 operon driven by the natural promoter was described previously (Minion *et al.*, 1989, *J Bacteriol* 165:1033-6).

The *E. coli* strain C600 (Sambrook *et al.*, *Molecular Cloning: A Laboratory Manual*, 2<sup>nd</sup> ed., Cold Spring Harbor Laboratory Press, New York (1989)) was used in this study. All bacteria used were grown in Luria Broth (LB) with appropriate antibiotics. Periplasmic extracts were isolated as described (Slonim *et al.*, 1992, *EMBO J.* 11:4747-56). Bacterial strain C600/pHJ9205 transformed with FimH expression constructs was used to produce large quantities of FimH proteins. These transformants were grown in LB in the presence of 0.1% arabinose and 0.1 mM IPTG to induce FimC and FimH expression, respectively. The protocol for the purification of FimCH complexes from bacterial periplasm has been described previously and was followed in this study (Barnhart *et al.*, 2000, *Proc. Natl. Acad. Sci. USA* 97:7670-2), which is hereby incorporated by reference in its entirety. Purified FimCH



complexes were dialyzed into 20 mM MES, pH 6.8 and stored at 4 °C.

### 6.6.2 Preparation Of FimCH - $\alpha$ -D-Mannopyranoside Co-Crystals

5 The FimCH complex was co-crystallized with  $\alpha$ -D-mannopyranoside by vapor diffusion in 4 ml hanging drops. 2 ml of FimCH at OD 5.9 (4.7 mg/ml) in 20 mM MES pH 6.5 and 7 mM  $\alpha$ -D-mannose was mixed with 2 ml of 1.0 M  $(\text{NH}_4)_2\text{SO}_4$  and 100 mM TRIS-HCl pH 8.2 and equilibrated against the latter solution. After 1 week the drops were streak seeded from drops containing small crystalline FimCH. Single bipyramidal crystals about 0.4 mm large in each dimension were fully grown after 2 weeks. The crystals were frozen in 10 after sequentially washing in 1.2 M  $(\text{NH}_4)_2\text{SO}_4$ , 100 mM Tris pH 8.2 complemented up to a final 25 % glycerol in steps of 5% glycerol.

### 6.6.3 Analysis And Characterization Of FimCH - $\alpha$ -D-Mannopyranoside Co-Crystals

#### 15 Diffraction Data Collection

Diffraction data sets were collected at beamline 19BM at Advanced Photon Source, Argonne, USA. Processing of the data was performed with an HKL2000 (Otwinowski & Minor, 1997, *Methods in Enzymology* 276:307-326). The crystals were frozen after sequentially soaking in 5% up to a final 25 % glycerol in 1.2 M  $(\text{NH}_4)_2\text{SO}_4$  and 100 mM Tris 20 pH 8.2. The space group was C2 with strong pseudotetragonal features. Unit cell dimensions were  $a=138.077$ ,  $b=138.130$ ,  $c=215.352$ ,  $\beta=90.005$  for FimCH mannose.

#### Structure Determination

Rigid body refinement was performed using the FimCH structure (PDB entry 25 code 1QUN) as the model. The refinement was started using a high temperature (3500 K) slowcool stage to remove model bias. Subsequent positional and individual B-factor refinements were performed without  $s$  cut-off, using CNS (Brunger *et al.*, 1998, *Acta Crystallogr D Biol Crystallogr.* 54:905-21). At this stage, electron densities were inspected and four of the eight molecules in the asymmetric unit were found to have good electron 30 density, in contrast with their four non-crystallographically related partners that had a significant part of the pilin domain of the adhesin and the chaperon disordered. The electron density of the receptor binding domain of the adhesin of all eight of the FimCH molecules was clearly defined and showed a mannoside in the carbohydrate binding pocket. Refinement and model building led to final  $R_{\text{free}}$  and  $R$  factors of 0.279 and 0.239 ( $50 - 2.8 \text{ \AA}$ ) for FimCH 35 mannose.



### Structure Analyses

Table 13 summarizes the X-ray crystallography refinement parameters of the structure of the crystalline FimCH -  $\alpha$ -D-mannopyranoside co-complex of the invention.

5	<u>Table 13</u> <u>Data Collection and Refinement Summary</u>		
	<u>space group</u>	<u>C2</u>	
	<u>unit cell</u>	<u>a (Å)</u>	<u>138.077</u>
		<u>b (Å)</u>	<u>138.130</u>
		<u>c (Å)</u>	<u>215.352</u>
		<u><math>\beta</math> (°)</u>	<u>90.005</u>
10	<u>Molecules per asymmetric unit</u>		<u>8</u>
	<u>Resolution</u>		<u>50.0 – 2.8</u>
	<u>number of observed reflections</u>		<u>370.427</u>
	<u>number of unique reflections</u>		<u>99.138</u>
	<u>highest resolution shell</u>		<u>2.9-2.8</u>
	<u>R-merge (%)</u>		<u>6.9 (47.8)</u>
15	<u>completeness (%)</u>		<u>99.8 (99.9)</u>
	<u><math>\langle I/\sigma(I) \rangle</math></u>		<u>13 (2.7)</u>
	<u>reflections with <math>I &gt; 2\sigma</math></u>		<u>83.8 (52.4)</u>
	<u>Number of protein atoms</u>		<u>29.168</u>
	<u>Number of water molecules</u>		<u>636</u>
	<u>sigma cut-off used in refinement</u>		<u>None</u>
	<u>crystallographic R-factor</u>		<u>0.239 (0.35)</u>
20	<u><math>R_{\text{free}}</math></u>		<u>0.279 (0.42)</u>
	<u>r.m.s. bond lengths (Å)</u>		<u>0.007</u>
	<u>r.m.s. bond angles (deg.)</u>		<u>1.4</u>

Table 14 provides the atomic structure coordinates of the crystalline FimCH -  $\alpha$ -D-mannopyranoside co-complex in Protein Database Format. The amino acid residue numbers coincide with those used in Figure 2.

Structures coordinates for the crystalline FimCH -  $\alpha$ -D-mannopyranoside co-complex according to Table 13 may be modified by mathematical manipulation. Such manipulations include, but are not limited to, crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, inversion of the raw structure coordinates and any combination of the above.

#### **6.6.4 Mutant FimCH - $\alpha$ -D-Mannopyranoside Co-Crystals**

The structure of the FimCH complex containing the Q133N mutation, derived from crystals grown in the presence of methyl- $\alpha$ -D-mannopyranoside, shows binding of the receptor (Figure 19B). The electron density is strongest at positions C4, C5 and C6 of the



sugar. The  $\alpha$ -linked methyl group on the anomeric O1 of mannose points outwards away from the pocket and makes a hydrophobic contact with Tyr48 (at 3.7 Å). Asn133 does not link to O3 of the mannose. Interestingly, the Q133N mutation not only affects the interactions originally made by Gln133, but the mannose also loses interaction with Asp140 and Asn135 (Figure 19). The mannose has shifted 0.7 Å from its position in the wild type. A shift in the protein backbone at Asp140 of about 0.7 Å together with changes in the side chain conformations of the Asn133, Asn135, Asn138 and Asp140 enables these residues to take part in a very different hydrogen bonding network (Figure 19B) than was present in the wild type FimCH-mannose structure (Figure 19A). This new hydrogen bonding network includes a new water molecule, W2, that interacts directly with O3. In contrast, the O2 ligand residues remained conserved including W1. W1 interacts both with O2 and the amide group of amino acid 133, as in the wild type complex. The hydrophobic part of the Gln133 side chain makes close van der Waals contacts with the Phe1 aromatic ring (Figure 19A). The shorter Asn133 side chain compensates for the lack of the penultimate carbon C $\gamma$  of Gln133 by establishing an amino-aromatic stacking interaction: Asn133 points its amide nitrogen atom towards the Phe1 ring (Figure 19B). Phe1 further stacks with Phe144. These stacking interactions in the  $\beta$ -strands holding the loop between Gln133 and Phe142 support the bottom part of the binding site formed by Asn46, Asp47 and Asp54. These results therefore explain how mutating a side chain can dramatically affect the structure of the mannose binding pocket.



Table 15  
Data Collection and Refinement Summary

	<u>space group</u>	<u>C2</u>
	<u>unit cell</u>	
	<u>a (Å)</u>	<u>138.349</u>
	<u>b (Å)</u>	<u>138.334</u>
5	<u>c (Å)</u>	<u>213.212</u>
	<u>β (°)</u>	<u>89.983</u>
	<u>Molecules per asymmetric unit</u>	<u>8</u>
	<u>Resolution</u>	<u>45-3.0</u>
	<u>number of observed reflections</u>	<u>197.848</u>
	<u>number of unique reflections</u>	<u>72.289</u>
	<u>highest resolution shell</u>	<u>3.11-3.0</u>
10	<u>R-merge (%)</u>	<u>8.7 (51.0)</u>
	<u>completeness (%)</u>	<u>87.1 (65.9)</u>
	<u>&lt;I/s(I)&gt;</u>	<u>10.6</u>
	<u>reflections with I &gt; 2</u>	<u>82.3 (60.8)</u>
	<u>Number of protein atoms</u>	<u>29,160</u>
	<u>Number of water molecules</u>	<u>377</u>
	<u>sigma cut-off used in refinement</u>	<u>None</u>
15	<u>crystallographic R-factor</u>	<u>0.236 (0.36)</u>
	<u>R<sub>free</sub></u>	<u>0.280 (0.39)</u>
	<u>r.m.s. bond lengths (Å)</u>	<u>0.007</u>
	<u>r.m.s. bond angles (deg.)</u>	<u>1.3</u>

Table 16 provides the atomic structure coordinates of the crystalline FimCH Q133N - α-D-mannopyranoside co-complex in Protein Database Format. The amino acid residue numbers coincide with those used in Figure 19.

Structures coordinates for the crystalline FimCH -α-D-mannopyranoside co-complex according to Table 15 may be modified by mathematical manipulation. Such manipulations include, but are not limited to, crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, inversion of the raw structure coordinates and any combination of the above.

#### Equivalents

Those skilled in the art will recognize, or be able to ascertain using no more than routine experimentation, many equivalents to the specific embodiments of the invention described herein. Such equivalents are intended to be encompassed by the following claims. without undue experimentation, to make such substitutions as will optimally serve their purposes in using the methods and procedures disclosed herein.



Table 14

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REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 45.0 - 2.79 A
REMARK starting r= 0.2400 free_r= 0.2781
REMARK final    r= 0.2393 free_r= 0.2788
REMARK rmsd bonds= 0.007084 rmsd angles= 1.39839
REMARK B rmsd for bonded mainchain atoms= 2.296 target= 2.0
REMARK B rmsd for bonded sidechain atoms= 3.458 target= 3.5
REMARK B rmsd for angle mainchain atoms= 3.912 target= 3.5
REMARK B rmsd for angle sidechain atoms= 4.836 target= 4.0
REMARK target= mlf final wa= 4.53034
REMARK final rweight= 0.0917 (with wa= 4.53034)
REMARK cycles= 2 coordinate steps= 30 B-factor steps= 30
REMARK sg= C2 a= 138.077 b= 138.130 c= 215.352 alpha= 90.000 beta= 90.005 gamma=
90.000
REMARK topology file 1 : CNS_TOPPAR:protein.top
REMARK topology file 2 : CNS_TOPPAR:dna-rna.top
REMARK topology file 3 : CNS_TOPPAR:water.top
REMARK topology file 4 : CNS_TOPPAR:ion.top
REMARK topology file 5 : CNS_TOPPAR:carbohydrate.top
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 3 : CNS_TOPPAR:water_rep.param
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : CNS_TOPPAR:carbohydrate.param
REMARK molecular structure file: water_pick6.mtf
REMARK input coordinates: ref14water6.pdb
REMARK reflection file= chwt35dman_batch2_C2.cv
REMARK ncs= restrain ncs file= ncs.def
REMARK B-correction resolution: 8.0 - 2.79
REMARK initial B-factor correction applied to fobs :
REMARK B11= 1.259 B22= 2.899 B33= -4.158
REMARK B12= 0.000 B13= 0.000 B23= 0.000
REMARK B-factor correction applied to coordinate array B: 1.274
REMARK bulk solvent: density level= 0.319338 e/A^3, B-factor= 66.2774 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 100483 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0): 1348 ( 1.3 % )
REMARK number of reflections rejected: 0 ( 0.0 % )
REMARK total number of reflections used: 99135 ( 98.7 % )
REMARK number of reflections in working set: 89199 ( 88.8 % )
REMARK number of reflections in test set: 9936 ( 9.9 % )
CRYST1 138.077 138.130 215.352 90.00 90.00 90.00 C 2
REMARK FILENAME="refine15_mlf.pdb"
REMARK DATE:04-May-01 07:53:09 created by user:
REMARK VERSION:1.0
ATOM 1 C GLY A 1 44.573 13.325 36.795 1.00 50.79 A
ATOM 2 O GLY A 1 45.727 13.137 36.430 1.00 53.80 A
ATOM 3 N GLY A 1 44.144 15.634 37.392 1.00 51.83 A
ATOM 4 CA GLY A 1 43.847 14.586 36.389 1.00 51.84 A
ATOM 5 N VAL A 2 43.915 12.471 37.571 1.00 45.13 A
ATOM 6 CA VAL A 2 44.533 11.231 38.004 1.00 37.93 A
ATOM 7 CB VAL A 2 44.363 11.029 39.510 1.00 36.03 A
ATOM 8 CG1 VAL A 2 44.840 9.652 39.889 1.00 41.26 A
ATOM 9 CG2 VAL A 2 45.155 12.087 40.273 1.00 30.35 A

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ATOM	10	C	VAL	A	2	43.883	10.081	37.256	1.00	38.28	A
ATOM	11	O	VAL	A	2	42.659	9.966	37.238	1.00	40.70	A
ATOM	12	N	ALA	A	3	44.699	9.234	36.625	1.00	38.38	A
ATOM	13	CA	ALA	A	3	44.162	8.111	35.852	1.00	34.00	A
ATOM	14	CB	ALA	A	3	44.263	8.408	34.383	1.00	29.35	A
ATOM	15	C	ALA	A	3	44.781	6.763	36.132	1.00	31.29	A
ATOM	16	O	ALA	A	3	45.969	6.652	36.389	1.00	35.76	A
ATOM	17	N	LEU	A	4	43.948	5.735	36.092	1.00	30.26	A
ATOM	18	CA	LEU	A	4	44.409	4.381	36.310	1.00	30.36	A
ATOM	19	CB	LEU	A	4	43.248	3.485	36.724	1.00	30.63	A
ATOM	20	CG	LEU	A	4	42.519	3.868	38.004	1.00	26.03	A
ATOM	21	CD1	LEU	A	4	41.555	2.748	38.400	1.00	22.68	A
ATOM	22	CD2	LEU	A	4	43.528	4.116	39.087	1.00	24.80	A
ATOM	23	C	LEU	A	4	44.983	3.882	34.992	1.00	32.66	A
ATOM	24	O	LEU	A	4	44.537	4.318	33.915	1.00	31.47	A
ATOM	25	N	GLY	A	5	45.954	2.967	35.088	1.00	31.82	A
ATOM	26	CA	GLY	A	5	46.607	2.400	33.915	1.00	26.34	A
ATOM	27	C	GLY	A	5	45.895	1.217	33.286	1.00	29.91	A
ATOM	28	O	GLY	A	5	46.403	0.617	32.351	1.00	37.42	A
ATOM	29	N	ALA	A	6	44.723	0.864	33.792	1.00	30.92	A
ATOM	30	CA	ALA	A	6	43.953	-0.243	33.228	1.00	32.99	A
ATOM	31	CB	ALA	A	6	44.337	-1.545	33.895	1.00	28.43	A
ATOM	32	C	ALA	A	6	42.479	0.041	33.465	1.00	33.61	A
ATOM	33	O	ALA	A	6	42.138	0.818	34.348	1.00	42.05	A
ATOM	34	N	THR	A	7	41.606	-0.584	32.694	1.00	28.40	A
ATOM	35	CA	THR	A	7	40.184	-0.367	32.860	1.00	24.73	A
ATOM	36	CB	THR	A	7	39.478	-0.133	31.503	1.00	21.10	A
ATOM	37	OG1	THR	A	7	39.490	-1.335	30.716	1.00	14.28	A
ATOM	38	CG2	THR	A	7	40.168	1.004	30.737	1.00	19.37	A
ATOM	39	C	THR	A	7	39.578	-1.573	33.538	1.00	29.26	A
ATOM	40	O	THR	A	7	38.359	-1.722	33.598	1.00	30.92	A
ATOM	41	N	ARG	A	8	40.447	-2.443	34.035	1.00	30.29	A
ATOM	42	CA	ARG	A	8	40.026	-3.654	34.739	1.00	30.40	A
ATOM	43	CB	ARG	A	8	39.248	-4.596	33.823	1.00	24.83	A
ATOM	44	CG	ARG	A	8	40.131	-5.428	32.911	1.00	29.92	A
ATOM	45	CD	ARG	A	8	39.806	-5.215	31.454	1.00	28.35	A
ATOM	46	NE	ARG	A	8	38.409	-5.525	31.149	1.00	27.35	A
ATOM	47	CZ	ARG	A	8	37.467	-4.606	30.944	1.00	24.04	A
ATOM	48	NH1	ARG	A	8	36.229	-4.980	30.672	1.00	21.41	A
ATOM	49	NH2	ARG	A	8	37.768	-3.316	30.997	1.00	12.41	A
ATOM	50	C	ARG	A	8	41.268	-4.374	35.271	1.00	30.62	A
ATOM	51	O	ARG	A	8	42.402	-4.060	34.906	1.00	31.02	A
ATOM	52	N	VAL	A	9	41.043	-5.346	36.138	1.00	28.47	A
ATOM	53	CA	VAL	A	9	42.127	-6.076	36.731	1.00	25.69	A
ATOM	54	CB	VAL	A	9	42.464	-5.512	38.106	1.00	20.88	A
ATOM	55	CG1	VAL	A	9	43.402	-6.428	38.823	1.00	29.03	A
ATOM	56	CG2	VAL	A	9	43.088	-4.156	37.951	1.00	20.94	A
ATOM	57	C	VAL	A	9	41.727	-7.524	36.880	1.00	29.36	A
ATOM	58	O	VAL	A	9	40.607	-7.838	37.295	1.00	27.18	A
ATOM	59	N	ILE	A	10	42.653	-8.401	36.507	1.00	31.47	A
ATOM	60	CA	ILE	A	10	42.437	-9.823	36.630	1.00	31.73	A
ATOM	61	CB	ILE	A	10	42.844	-10.553	35.374	1.00	24.79	A
ATOM	62	CG2	ILE	A	10	42.634	-12.034	35.554	1.00	22.18	A
ATOM	63	CG1	ILE	A	10	41.985	-10.060	34.217	1.00	28.91	A
ATOM	64	CD1	ILE	A	10	40.498	-10.358	34.363	1.00	22.28	A
ATOM	65	C	ILE	A	10	43.297	-10.295	37.775	1.00	35.17	A
ATOM	66	O	ILE	A	10	44.513	-10.155	37.735	1.00	34.50	A
ATOM	67	N	TYR	A	11	42.658	-10.821	38.812	1.00	38.03	A



ATOM	68	CA	TYR	A	11	43.396	-11.319	39.961	1.00	37.70	A
ATOM	69	CB	TYR	A	11	42.707	-10.949	41.266	1.00	35.50	A
ATOM	70	CG	TYR	A	11	43.651	-10.957	42.435	1.00	39.89	A
ATOM	71	CD1	TYR	A	11	44.292	-9.788	42.840	1.00	44.53	A
ATOM	72	CE1	TYR	A	11	45.213	-9.785	43.883	1.00	42.70	A
ATOM	73	CD2	TYR	A	11	43.950	-12.135	43.107	1.00	37.58	A
ATOM	74	CE2	TYR	A	11	44.876	-12.144	44.156	1.00	41.09	A
ATOM	75	CZ	TYR	A	11	45.504	-10.961	44.535	1.00	41.23	A
ATOM	76	OH	TYR	A	11	46.441	-10.942	45.544	1.00	37.92	A
ATOM	77	C	TYR	A	11	43.452	-12.830	39.857	1.00	37.01	A
ATOM	78	O	TYR	A	11	42.436	-13.498	40.048	1.00	30.91	A
ATOM	79	N	PRO	A	12	44.641	-13.385	39.534	1.00	39.74	A
ATOM	80	CD	PRO	A	12	45.850	-12.640	39.145	1.00	41.45	A
ATOM	81	CA	PRO	A	12	44.870	-14.831	39.396	1.00	37.85	A
ATOM	82	CB	PRO	A	12	46.270	-14.911	38.784	1.00	36.62	A
ATOM	83	CG	PRO	A	12	46.460	-13.558	38.135	1.00	40.43	A
ATOM	84	C	PRO	A	12	44.834	-15.476	40.763	1.00	36.08	A
ATOM	85	O	PRO	A	12	45.631	-15.121	41.627	1.00	35.11	A
ATOM	86	N	ALA	A	13	43.909	-16.406	40.974	1.00	39.36	A
ATOM	87	CA	ALA	A	13	43.824	-17.067	42.268	1.00	45.24	A
ATOM	88	CB	ALA	A	13	42.778	-18.162	42.232	1.00	45.78	A
ATOM	89	C	ALA	A	13	45.196	-17.648	42.611	1.00	50.96	A
ATOM	90	O	ALA	A	13	45.799	-18.372	41.810	1.00	53.35	A
ATOM	91	N	GLY	A	14	45.696	-17.306	43.795	1.00	53.38	A
ATOM	92	CA	GLY	A	14	46.991	-17.801	44.211	1.00	53.63	A
ATOM	93	C	GLY	A	14	48.012	-16.690	44.314	1.00	56.81	A
ATOM	94	O	GLY	A	14	48.766	-16.635	45.286	1.00	56.45	A
ATOM	95	N	GLN	A	15	48.048	-15.809	43.313	1.00	57.74	A
ATOM	96	CA	GLN	A	15	48.994	-14.697	43.307	1.00	58.70	A
ATOM	97	CB	GLN	A	15	48.621	-13.682	42.228	1.00	62.60	A
ATOM	98	CG	GLN	A	15	48.488	-14.259	40.834	1.00	70.57	A
ATOM	99	CD	GLN	A	15	49.757	-14.154	40.013	1.00	74.96	A
ATOM	100	OE1	GLN	A	15	50.828	-14.585	40.441	1.00	78.07	A
ATOM	101	NE2	GLN	A	15	49.639	-13.585	38.815	1.00	77.11	A
ATOM	102	C	GLN	A	15	48.969	-14.010	44.665	1.00	60.62	A
ATOM	103	O	GLN	A	15	47.905	-13.786	45.242	1.00	61.49	A
ATOM	104	N	LYS	A	16	50.140	-13.679	45.182	1.00	62.37	A
ATOM	105	CA	LYS	A	16	50.202	-13.015	46.469	1.00	65.91	A
ATOM	106	CB	LYS	A	16	51.638	-12.968	46.977	1.00	72.82	A
ATOM	107	CG	LYS	A	16	51.774	-12.473	48.410	1.00	80.90	A
ATOM	108	CD	LYS	A	16	53.238	-12.265	48.796	1.00	86.89	A
ATOM	109	CE	LYS	A	16	54.125	-13.434	48.345	1.00	88.82	A
ATOM	110	NZ	LYS	A	16	53.660	-14.763	48.844	1.00	90.38	A
ATOM	111	C	LYS	A	16	49.676	-11.597	46.316	1.00	64.89	A
ATOM	112	O	LYS	A	16	49.138	-11.022	47.259	1.00	67.77	A
ATOM	113	N	GLN	A	17	49.821	-11.040	45.118	1.00	61.76	A
ATOM	114	CA	GLN	A	17	49.371	-9.677	44.864	1.00	58.78	A
ATOM	115	CB	GLN	A	17	50.213	-8.708	45.684	1.00	57.80	A
ATOM	116	CG	GLN	A	17	51.678	-8.860	45.396	1.00	62.19	A
ATOM	117	CD	GLN	A	17	52.461	-7.602	45.661	1.00	68.02	A
ATOM	118	OE1	GLN	A	17	52.472	-7.086	46.789	1.00	67.38	A
ATOM	119	NE2	GLN	A	17	53.135	-7.092	44.618	1.00	63.55	A
ATOM	120	C	GLN	A	17	49.452	-9.260	43.394	1.00	54.17	A
ATOM	121	O	GLN	A	17	50.321	-9.709	42.656	1.00	54.89	A
ATOM	122	N	VAL	A	18	48.534	-8.398	42.975	1.00	49.56	A
ATOM	123	CA	VAL	A	18	48.536	-7.900	41.613	1.00	46.26	A
ATOM	124	CB	VAL	A	18	47.223	-8.194	40.906	1.00	45.25	A
ATOM	125	CG1	VAL	A	18	47.237	-7.586	39.519	1.00	44.64	A



ATOM	126	CG2	VAL	A	18	47.016	-9.685	40.815	1.00	46.03	A
ATOM	127	C	VAL	A	18	48.722	-6.397	41.729	1.00	48.04	A
ATOM	128	O	VAL	A	18	48.337	-5.794	42.729	1.00	50.94	A
ATOM	129	N	GLN	A	19	49.321	-5.782	40.723	1.00	45.47	A
ATOM	130	CA	GLN	A	19	49.544	-4.359	40.794	1.00	43.17	A
ATOM	131	CB	GLN	A	19	51.035	-4.081	40.886	1.00	46.44	A
ATOM	132	CG	GLN	A	19	51.860	-4.849	39.900	1.00	54.70	A
ATOM	133	CD	GLN	A	19	53.307	-4.938	40.329	1.00	57.93	A
ATOM	134	OE1	GLN	A	19	53.621	-5.548	41.354	1.00	63.32	A
ATOM	135	NE2	GLN	A	19	54.196	-4.324	39.556	1.00	60.14	A
ATOM	136	C	GLN	A	19	48.912	-3.578	39.660	1.00	39.45	A
ATOM	137	O	GLN	A	19	48.775	-4.074	38.554	1.00	38.04	A
ATOM	138	N	LEU	A	20	48.511	-2.350	39.981	1.00	34.78	A
ATOM	139	CA	LEU	A	20	47.857	-1.438	39.065	1.00	31.20	A
ATOM	140	CB	LEU	A	20	46.401	-1.244	39.508	1.00	26.86	A
ATOM	141	CG	LEU	A	20	45.467	-0.342	38.685	1.00	33.45	A
ATOM	142	CD1	LEU	A	20	45.196	-0.967	37.329	1.00	24.45	A
ATOM	143	CD2	LEU	A	20	44.151	-0.144	39.432	1.00	30.84	A
ATOM	144	C	LEU	A	20	48.610	-0.101	39.085	1.00	32.48	A
ATOM	145	O	LEU	A	20	49.136	0.313	40.117	1.00	32.34	A
ATOM	146	N	ALA	A	21	48.658	0.576	37.943	1.00	33.28	A
ATOM	147	CA	ALA	A	21	49.370	1.842	37.855	1.00	30.08	A
ATOM	148	CB	ALA	A	21	50.118	1.937	36.539	1.00	24.35	A
ATOM	149	C	ALA	A	21	48.432	3.009	37.972	1.00	31.45	A
ATOM	150	O	ALA	A	21	47.280	2.947	37.535	1.00	30.03	A
ATOM	151	N	VAL	A	22	48.945	4.075	38.571	1.00	32.81	A
ATOM	152	CA	VAL	A	22	48.194	5.299	38.747	1.00	34.61	A
ATOM	153	CB	VAL	A	22	47.844	5.608	40.196	1.00	32.97	A
ATOM	154	CG1	VAL	A	22	46.541	6.403	40.242	1.00	33.01	A
ATOM	155	CG2	VAL	A	22	47.783	4.353	40.997	1.00	34.95	A
ATOM	156	C	VAL	A	22	49.150	6.378	38.341	1.00	40.85	A
ATOM	157	O	VAL	A	22	50.331	6.357	38.709	1.00	43.10	A
ATOM	158	N	THR	A	23	48.631	7.341	37.605	1.00	42.34	A
ATOM	159	CA	THR	A	23	49.441	8.430	37.149	1.00	40.73	A
ATOM	160	CB	THR	A	23	49.854	8.189	35.698	1.00	42.89	A
ATOM	161	OG1	THR	A	23	50.298	9.418	35.118	1.00	54.11	A
ATOM	162	CG2	THR	A	23	48.689	7.646	34.901	1.00	47.21	A
ATOM	163	C	THR	A	23	48.635	9.708	37.290	1.00	38.53	A
ATOM	164	O	THR	A	23	47.448	9.733	36.992	1.00	35.79	A
ATOM	165	N	ASN	A	24	49.302	10.751	37.775	1.00	40.34	A
ATOM	166	CA	ASN	A	24	48.719	12.066	37.991	1.00	40.97	A
ATOM	167	CB	ASN	A	24	49.055	12.538	39.409	1.00	35.01	A
ATOM	168	CG	ASN	A	24	48.653	13.987	39.661	1.00	43.23	A
ATOM	169	OD1	ASN	A	24	47.764	14.517	38.999	1.00	38.96	A
ATOM	170	ND2	ASN	A	24	49.299	14.628	40.636	1.00	41.00	A
ATOM	171	C	ASN	A	24	49.273	13.047	36.958	1.00	47.73	A
ATOM	172	O	ASN	A	24	50.463	13.391	36.982	1.00	47.30	A
ATOM	173	N	ASN	A	25	48.396	13.483	36.056	1.00	52.99	A
ATOM	174	CA	ASN	A	25	48.726	14.421	34.976	1.00	56.93	A
ATOM	175	CB	ASN	A	25	47.571	14.509	33.977	1.00	55.68	A
ATOM	176	CG	ASN	A	25	47.319	13.215	33.263	1.00	53.81	A
ATOM	177	OD1	ASN	A	25	47.560	12.134	33.804	1.00	52.54	A
ATOM	178	ND2	ASN	A	25	46.810	13.310	32.040	1.00	56.02	A
ATOM	179	C	ASN	A	25	49.007	15.836	35.454	1.00	60.12	A
ATOM	180	O	ASN	A	25	50.047	16.412	35.146	1.00	63.46	A
ATOM	181	N	ASP	A	26	48.049	16.399	36.180	1.00	60.03	A
ATOM	182	CA	ASP	A	26	48.153	17.755	36.683	1.00	61.14	A
ATOM	183	CB	ASP	A	26	47.128	17.971	37.775	1.00	63.54	A



ATOM	184	CG	ASP	A	26	45.722	17.815	37.267	1.00	64.77	A
ATOM	185	OD1	ASP	A	26	44.792	17.913	38.093	1.00	67.45	A
ATOM	186	OD2	ASP	A	26	45.550	17.591	36.043	1.00	65.91	A
ATOM	187	C	ASP	A	26	49.521	18.147	37.180	1.00	62.42	A
ATOM	188	O	ASP	A	26	49.892	17.878	38.317	1.00	61.06	A
ATOM	189	N	GLU	A	27	50.256	18.809	36.302	1.00	67.35	A
ATOM	190	CA	GLU	A	27	51.600	19.265	36.592	1.00	71.48	A
ATOM	191	CB	GLU	A	27	52.070	20.198	35.468	1.00	78.88	A
ATOM	192	CG	GLU	A	27	52.499	19.441	34.200	1.00	92.01	A
ATOM	193	CD	GLU	A	27	52.239	20.197	32.899	1.00	97.34	A
ATOM	194	OE1	GLU	A	27	52.662	21.371	32.783	1.00	102.85	A
ATOM	195	OE2	GLU	A	27	51.619	19.602	31.985	1.00	99.30	A
ATOM	196	C	GLU	A	27	51.719	19.952	37.942	1.00	69.71	A
ATOM	197	O	GLU	A	27	52.804	20.009	38.506	1.00	69.50	A
ATOM	198	N	ASN	A	28	50.616	20.461	38.477	1.00	68.96	A
ATOM	199	CA	ASN	A	28	50.704	21.135	39.759	1.00	71.52	A
ATOM	200	CB	ASN	A	28	51.186	22.579	39.555	1.00	77.25	A
ATOM	201	CG	ASN	A	28	50.385	23.327	38.497	1.00	80.81	A
ATOM	202	OD1	ASN	A	28	50.786	24.402	38.043	1.00	80.59	A
ATOM	203	ND2	ASN	A	28	49.245	22.760	38.101	1.00	82.72	A
ATOM	204	C	ASN	A	28	49.422	21.112	40.562	1.00	70.70	A
ATOM	205	O	ASN	A	28	48.511	21.901	40.340	1.00	74.18	A
ATOM	206	N	SER	A	29	49.383	20.196	41.515	1.00	70.28	A
ATOM	207	CA	SER	A	29	48.245	19.999	42.405	1.00	69.73	A
ATOM	208	CB	SER	A	29	46.925	20.032	41.623	1.00	70.95	A
ATOM	209	OG	SER	A	29	46.897	19.035	40.618	1.00	69.06	A
ATOM	210	C	SER	A	29	48.442	18.621	43.034	1.00	66.59	A
ATOM	211	O	SER	A	29	48.460	17.610	42.338	1.00	66.98	A
ATOM	212	N	THR	A	30	48.613	18.581	44.346	1.00	62.94	A
ATOM	213	CA	THR	A	30	48.822	17.312	45.010	1.00	58.80	A
ATOM	214	CB	THR	A	30	49.488	17.515	46.376	1.00	60.11	A
ATOM	215	OG1	THR	A	30	50.669	18.313	46.221	1.00	60.81	A
ATOM	216	CG2	THR	A	30	49.903	16.189	46.957	1.00	65.77	A
ATOM	217	C	THR	A	30	47.497	16.590	45.189	1.00	55.15	A
ATOM	218	O	THR	A	30	46.431	17.197	45.103	1.00	57.03	A
ATOM	219	N	TYR	A	31	47.567	15.285	45.410	1.00	51.62	A
ATOM	220	CA	TYR	A	31	46.373	14.470	45.618	1.00	48.42	A
ATOM	221	CB	TYR	A	31	45.941	13.790	44.327	1.00	47.52	A
ATOM	222	CG	TYR	A	31	45.261	14.681	43.331	1.00	51.38	A
ATOM	223	CD1	TYR	A	31	45.867	14.994	42.113	1.00	50.92	A
ATOM	224	CE1	TYR	A	31	45.201	15.749	41.162	1.00	54.59	A
ATOM	225	CD2	TYR	A	31	43.975	15.153	43.570	1.00	53.90	A
ATOM	226	CE2	TYR	A	31	43.300	15.905	42.623	1.00	54.60	A
ATOM	227	CZ	TYR	A	31	43.916	16.196	41.425	1.00	56.01	A
ATOM	228	OH	TYR	A	31	43.234	16.912	40.479	1.00	63.46	A
ATOM	229	C	TYR	A	31	46.614	13.378	46.647	1.00	46.00	A
ATOM	230	O	TYR	A	31	47.735	12.910	46.845	1.00	48.20	A
ATOM	231	N	LEU	A	32	45.550	12.981	47.317	1.00	43.61	A
ATOM	232	CA	LEU	A	32	45.641	11.913	48.283	1.00	42.05	A
ATOM	233	CB	LEU	A	32	44.907	12.268	49.569	1.00	48.78	A
ATOM	234	CG	LEU	A	32	45.708	13.010	50.632	1.00	52.70	A
ATOM	235	CD1	LEU	A	32	44.766	13.447	51.753	1.00	53.82	A
ATOM	236	CD2	LEU	A	32	46.827	12.107	51.153	1.00	46.91	A
ATOM	237	C	LEU	A	32	44.934	10.770	47.599	1.00	43.83	A
ATOM	238	O	LEU	A	32	43.762	10.878	47.214	1.00	40.62	A
ATOM	239	N	ILE	A	33	45.660	9.682	47.417	1.00	42.76	A
ATOM	240	CA	ILE	A	33	45.088	8.525	46.775	1.00	38.12	A
ATOM	241	CB	ILE	A	33	46.139	7.822	45.911	1.00	36.49	A



ATOM	242	CG2	ILE	A	33	45.513	6.655	45.157	1.00	40.10	A
ATOM	243	CG1	ILE	A	33	46.762	8.846	44.959	1.00	38.79	A
ATOM	244	CD1	ILE	A	33	45.752	9.675	44.183	1.00	28.86	A
ATOM	245	C	ILE	A	33	44.591	7.598	47.859	1.00	35.40	A
ATOM	246	O	ILE	A	33	45.333	7.224	48.760	1.00	36.59	A
ATOM	247	N	GLN	A	34	43.321	7.249	47.770	1.00	33.93	A
ATOM	248	CA	GLN	A	34	42.688	6.358	48.730	1.00	35.55	A
ATOM	249	CB	GLN	A	34	41.659	7.135	49.539	1.00	40.32	A
ATOM	250	CG	GLN	A	34	41.417	6.623	50.923	1.00	41.00	A
ATOM	251	CD	GLN	A	34	40.494	7.533	51.692	1.00	45.44	A
ATOM	252	OE1	GLN	A	34	39.329	7.700	51.335	1.00	52.79	A
ATOM	253	NE2	GLN	A	34	41.013	8.145	52.746	1.00	47.22	A
ATOM	254	C	GLN	A	34	41.997	5.291	47.895	1.00	33.40	A
ATOM	255	O	GLN	A	34	41.079	5.594	47.143	1.00	32.21	A
ATOM	256	N	SER	A	35	42.431	4.045	48.036	1.00	32.83	A
ATOM	257	CA	SER	A	35	41.864	2.961	47.249	1.00	32.88	A
ATOM	258	CB	SER	A	35	42.968	2.340	46.398	1.00	38.87	A
ATOM	259	OG	SER	A	35	43.755	3.350	45.799	1.00	47.39	A
ATOM	260	C	SER	A	35	41.214	1.869	48.077	1.00	30.90	A
ATOM	261	O	SER	A	35	41.593	1.643	49.215	1.00	39.12	A
ATOM	262	N	TRP	A	36	40.240	1.182	47.502	1.00	25.03	A
ATOM	263	CA	TRP	A	36	39.580	0.082	48.198	1.00	25.04	A
ATOM	264	CB	TRP	A	36	38.594	0.587	49.257	1.00	18.25	A
ATOM	265	CG	TRP	A	36	37.338	1.180	48.706	1.00	20.02	A
ATOM	266	CD2	TRP	A	36	37.158	2.524	48.248	1.00	16.95	A
ATOM	267	CE2	TRP	A	36	35.827	2.630	47.772	1.00	22.43	A
ATOM	268	CE3	TRP	A	36	37.989	3.650	48.198	1.00	11.35	A
ATOM	269	CD1	TRP	A	36	36.151	0.540	48.497	1.00	21.69	A
ATOM	270	NE1	TRP	A	36	35.235	1.404	47.936	1.00	24.21	A
ATOM	271	CZ2	TRP	A	36	35.303	3.829	47.247	1.00	17.19	A
ATOM	272	CZ3	TRP	A	36	37.465	4.857	47.678	1.00	15.18	A
ATOM	273	CH2	TRP	A	36	36.132	4.931	47.212	1.00	10.97	A
ATOM	274	C	TRP	A	36	38.853	-0.797	47.189	1.00	25.22	A
ATOM	275	O	TRP	A	36	38.759	-0.476	46.007	1.00	24.89	A
ATOM	276	N	VAL	A	37	38.343	-1.915	47.666	1.00	24.80	A
ATOM	277	CA	VAL	A	37	37.654	-2.836	46.805	1.00	26.60	A
ATOM	278	CB	VAL	A	37	38.524	-4.070	46.531	1.00	28.07	A
ATOM	279	CG1	VAL	A	37	37.783	-5.034	45.631	1.00	29.46	A
ATOM	280	CG2	VAL	A	37	39.828	-3.640	45.893	1.00	26.19	A
ATOM	281	C	VAL	A	37	36.358	-3.279	47.452	1.00	26.97	A
ATOM	282	O	VAL	A	37	36.353	-3.783	48.571	1.00	32.49	A
ATOM	283	N	GLU	A	38	35.263	-3.086	46.737	1.00	22.36	A
ATOM	284	CA	GLU	A	38	33.958	-3.484	47.218	1.00	25.19	A
ATOM	285	CB	GLU	A	38	32.929	-2.426	46.850	1.00	23.47	A
ATOM	286	CG	GLU	A	38	33.247	-1.083	47.474	1.00	29.25	A
ATOM	287	CD	GLU	A	38	32.394	0.013	46.925	1.00	31.37	A
ATOM	288	OE1	GLU	A	38	31.336	-0.340	46.357	1.00	33.29	A
ATOM	289	OE2	GLU	A	38	32.769	1.208	47.067	1.00	29.73	A
ATOM	290	C	GLU	A	38	33.650	-4.782	46.515	1.00	27.91	A
ATOM	291	O	GLU	A	38	34.249	-5.077	45.482	1.00	30.92	A
ATOM	292	N	ASN	A	39	32.751	-5.578	47.082	1.00	27.23	A
ATOM	293	CA	ASN	A	39	32.397	-6.825	46.438	1.00	28.78	A
ATOM	294	CB	ASN	A	39	31.982	-7.889	47.451	1.00	31.06	A
ATOM	295	CG	ASN	A	39	30.711	-7.533	48.199	1.00	41.12	A
ATOM	296	OD1	ASN	A	39	29.906	-6.709	47.749	1.00	41.67	A
ATOM	297	ND2	ASN	A	39	30.513	-8.176	49.344	1.00	42.07	A
ATOM	298	C	ASN	A	39	31.262	-6.551	45.467	1.00	30.36	A
ATOM	299	O	ASN	A	39	30.858	-5.403	45.288	1.00	28.38	A



ATOM	300	N	ALA	A	40	30.748	-7.613	44.852	1.00	33.88	A
ATOM	301	CA	ALA	A	40	29.691	-7.489	43.867	1.00	32.53	A
ATOM	302	CB	ALA	A	40	29.265	-8.847	43.402	1.00	36.04	A
ATOM	303	C	ALA	A	40	28.502	-6.716	44.375	1.00	34.18	A
ATOM	304	O	ALA	A	40	27.903	-5.952	43.634	1.00	37.55	A
ATOM	305	N	ASP	A	41	28.154	-6.897	45.638	1.00	35.10	A
ATOM	306	CA	ASP	A	41	27.018	-6.172	46.172	1.00	40.17	A
ATOM	307	CB	ASP	A	41	26.436	-6.907	47.367	1.00	46.82	A
ATOM	308	CG	ASP	A	41	25.760	-8.197	46.967	1.00	51.21	A
ATOM	309	OD1	ASP	A	41	24.921	-8.152	46.045	1.00	54.74	A
ATOM	310	OD2	ASP	A	41	26.062	-9.247	47.569	1.00	49.46	A
ATOM	311	C	ASP	A	41	27.314	-4.731	46.548	1.00	41.50	A
ATOM	312	O	ASP	A	41	26.434	-4.026	47.017	1.00	47.75	A
ATOM	313	N	GLY	A	42	28.546	-4.287	46.340	1.00	38.41	A
ATOM	314	CA	GLY	A	42	28.880	-2.915	46.654	1.00	31.80	A
ATOM	315	C	GLY	A	42	29.339	-2.711	48.073	1.00	31.58	A
ATOM	316	O	GLY	A	42	29.633	-1.591	48.461	1.00	32.94	A
ATOM	317	N	VAL	A	43	29.415	-3.772	48.864	1.00	33.94	A
ATOM	318	CA	VAL	A	43	29.857	-3.585	50.235	1.00	36.76	A
ATOM	319	CB	VAL	A	43	29.086	-4.505	51.225	1.00	31.92	A
ATOM	320	CG1	VAL	A	43	27.956	-5.203	50.524	1.00	32.27	A
ATOM	321	CG2	VAL	A	43	30.021	-5.481	51.878	1.00	34.85	A
ATOM	322	C	VAL	A	43	31.366	-3.770	50.406	1.00	40.26	A
ATOM	323	O	VAL	A	43	31.984	-4.648	49.782	1.00	40.24	A
ATOM	324	N	LYS	A	44	31.950	-2.922	51.252	1.00	38.14	A
ATOM	325	CA	LYS	A	44	33.372	-2.977	51.510	1.00	38.87	A
ATOM	326	CB	LYS	A	44	33.873	-1.658	52.115	1.00	38.71	A
ATOM	327	CG	LYS	A	44	33.689	-0.406	51.277	1.00	38.64	A
ATOM	328	CD	LYS	A	44	32.808	0.593	51.997	1.00	45.19	A
ATOM	329	CE	LYS	A	44	32.660	1.863	51.211	1.00	44.21	A
ATOM	330	NZ	LYS	A	44	33.992	2.459	51.006	1.00	53.47	A
ATOM	331	C	LYS	A	44	33.729	-4.101	52.472	1.00	40.34	A
ATOM	332	O	LYS	A	44	33.903	-3.864	53.668	1.00	41.16	A
ATOM	333	N	ASP	A	45	33.796	-5.334	51.988	1.00	41.72	A
ATOM	334	CA	ASP	A	45	34.236	-6.399	52.879	1.00	42.88	A
ATOM	335	CB	ASP	A	45	33.736	-7.766	52.441	1.00	45.54	A
ATOM	336	CG	ASP	A	45	33.828	-7.973	50.952	1.00	45.53	A
ATOM	337	OD1	ASP	A	45	34.746	-7.404	50.328	1.00	46.24	A
ATOM	338	OD2	ASP	A	45	32.983	-8.722	50.416	1.00	39.44	A
ATOM	339	C	ASP	A	45	35.739	-6.311	52.728	1.00	46.78	A
ATOM	340	O	ASP	A	45	36.246	-5.430	52.019	1.00	52.22	A
ATOM	341	N	GLY	A	46	36.477	-7.204	53.355	1.00	46.85	A
ATOM	342	CA	GLY	A	46	37.917	-7.067	53.229	1.00	44.85	A
ATOM	343	C	GLY	A	46	38.525	-8.097	52.322	1.00	43.84	A
ATOM	344	O	GLY	A	46	39.712	-8.393	52.444	1.00	42.91	A
ATOM	345	N	ARG	A	47	37.718	-8.641	51.412	1.00	41.43	A
ATOM	346	CA	ARG	A	47	38.204	-9.659	50.507	1.00	39.36	A
ATOM	347	CB	ARG	A	47	37.149	-9.990	49.473	1.00	48.60	A
ATOM	348	CG	ARG	A	47	36.523	-11.347	49.699	1.00	59.40	A
ATOM	349	CD	ARG	A	47	35.682	-11.368	50.952	1.00	67.93	A
ATOM	350	NE	ARG	A	47	35.210	-12.718	51.234	1.00	81.01	A
ATOM	351	CZ	ARG	A	47	35.960	-13.664	51.793	1.00	88.24	A
ATOM	352	NH1	ARG	A	47	37.213	-13.398	52.135	1.00	92.78	A
ATOM	353	NH2	ARG	A	47	35.468	-14.880	52.005	1.00	91.41	A
ATOM	354	C	ARG	A	47	39.498	-9.260	49.828	1.00	38.41	A
ATOM	355	O	ARG	A	47	40.374	-10.092	49.608	1.00	36.37	A
ATOM	356	N	PHE	A	48	39.633	-7.983	49.504	1.00	35.37	A
ATOM	357	CA	PHE	A	48	40.851	-7.518	48.862	1.00	35.98	A



ATOM	358	CB	PHE	A	48	40.635	-7.303	47.352	1.00	33.65	A
ATOM	359	CG	PHE	A	48	40.439	-8.571	46.602	1.00	31.31	A
ATOM	360	CD1	PHE	A	48	39.172	-9.129	46.481	1.00	33.95	A
ATOM	361	CD2	PHE	A	48	41.537	-9.272	46.109	1.00	32.43	A
ATOM	362	CE1	PHE	A	48	39.000	-10.378	45.891	1.00	32.81	A
ATOM	363	CE2	PHE	A	48	41.383	-10.514	45.520	1.00	31.82	A
ATOM	364	CZ	PHE	A	48	40.116	-11.077	45.409	1.00	30.28	A
ATOM	365	C	PHE	A	48	41.320	-6.237	49.512	1.00	34.18	A
ATOM	366	O	PHE	A	48	40.505	-5.423	49.906	1.00	31.01	A
ATOM	367	N	ILE	A	49	42.635	-6.061	49.609	1.00	35.45	A
ATOM	368	CA	ILE	A	49	43.191	-4.871	50.225	1.00	36.92	A
ATOM	369	CB	ILE	A	49	43.813	-5.224	51.582	1.00	42.20	A
ATOM	370	CG2	ILE	A	49	44.465	-4.001	52.221	1.00	35.45	A
ATOM	371	CG1	ILE	A	49	42.701	-5.733	52.499	1.00	44.49	A
ATOM	372	CD1	ILE	A	49	43.201	-6.508	53.688	1.00	53.29	A
ATOM	373	C	ILE	A	49	44.209	-4.245	49.304	1.00	35.56	A
ATOM	374	O	ILE	A	49	45.009	-4.933	48.685	1.00	39.65	A
ATOM	375	N	VAL	A	50	44.175	-2.927	49.215	1.00	32.29	A
ATOM	376	CA	VAL	A	50	45.071	-2.211	48.330	1.00	33.81	A
ATOM	377	CB	VAL	A	50	44.279	-1.218	47.435	1.00	35.53	A
ATOM	378	CG1	VAL	A	50	45.207	-0.573	46.421	1.00	37.38	A
ATOM	379	CG2	VAL	A	50	43.125	-1.937	46.741	1.00	37.16	A
ATOM	380	C	VAL	A	50	46.067	-1.423	49.143	1.00	35.47	A
ATOM	381	O	VAL	A	50	45.720	-0.887	50.188	1.00	39.81	A
ATOM	382	N	THR	A	51	47.304	-1.351	48.671	1.00	35.54	A
ATOM	383	CA	THR	A	51	48.327	-0.580	49.365	1.00	34.50	A
ATOM	384	CB	THR	A	51	49.338	-1.464	50.123	1.00	37.75	A
ATOM	385	OG1	THR	A	51	49.924	-2.404	49.213	1.00	44.60	A
ATOM	386	CG2	THR	A	51	48.677	-2.205	51.261	1.00	46.16	A
ATOM	387	C	THR	A	51	49.122	0.214	48.350	1.00	34.70	A
ATOM	388	O	THR	A	51	49.304	-0.209	47.211	1.00	35.22	A
ATOM	389	N	PRO	A	52	49.561	1.406	48.738	1.00	34.51	A
ATOM	390	CD	PRO	A	52	50.735	2.071	48.158	1.00	30.64	A
ATOM	391	CA	PRO	A	52	49.274	1.930	50.075	1.00	34.32	A
ATOM	392	CB	PRO	A	52	50.259	3.090	50.220	1.00	32.25	A
ATOM	393	CG	PRO	A	52	50.667	3.407	48.819	1.00	36.50	A
ATOM	394	C	PRO	A	52	47.832	2.392	50.157	1.00	34.16	A
ATOM	395	O	PRO	A	52	47.312	2.991	49.223	1.00	39.05	A
ATOM	396	N	PRO	A	53	47.161	2.115	51.275	1.00	32.08	A
ATOM	397	CD	PRO	A	53	47.651	1.487	52.513	1.00	27.65	A
ATOM	398	CA	PRO	A	53	45.765	2.538	51.410	1.00	30.20	A
ATOM	399	CB	PRO	A	53	45.386	2.020	52.790	1.00	31.39	A
ATOM	400	CG	PRO	A	53	46.713	2.043	53.534	1.00	21.96	A
ATOM	401	C	PRO	A	53	45.552	4.047	51.286	1.00	30.89	A
ATOM	402	O	PRO	A	53	44.445	4.490	51.000	1.00	30.55	A
ATOM	403	N	LEU	A	54	46.610	4.830	51.499	1.00	32.19	A
ATOM	404	CA	LEU	A	54	46.525	6.290	51.434	1.00	32.42	A
ATOM	405	CB	LEU	A	54	45.980	6.838	52.737	1.00	35.06	A
ATOM	406	CG	LEU	A	54	45.866	8.355	52.833	1.00	35.56	A
ATOM	407	CD1	LEU	A	54	44.602	8.812	52.104	1.00	39.67	A
ATOM	408	CD2	LEU	A	54	45.807	8.757	54.291	1.00	34.78	A
ATOM	409	C	LEU	A	54	47.883	6.920	51.222	1.00	35.61	A
ATOM	410	O	LEU	A	54	48.789	6.720	52.035	1.00	40.67	A
ATOM	411	N	PHE	A	55	48.028	7.705	50.162	1.00	33.82	A
ATOM	412	CA	PHE	A	55	49.313	8.339	49.878	1.00	36.60	A
ATOM	413	CB	PHE	A	55	50.263	7.343	49.227	1.00	35.58	A
ATOM	414	CG	PHE	A	55	49.797	6.856	47.895	1.00	40.56	A
ATOM	415	CD1	PHE	A	55	50.227	7.467	46.720	1.00	42.70	A



ATOM	416	CD2	PHE	A	55	48.903	5.799	47.813	1.00	44.00	A
ATOM	417	CE1	PHE	A	55	49.768	7.029	45.471	1.00	46.06	A
ATOM	418	CE2	PHE	A	55	48.435	5.352	46.575	1.00	50.94	A
ATOM	419	CZ	PHE	A	55	48.869	5.969	45.397	1.00	48.90	A
ATOM	420	C	PHE	A	55	49.160	9.534	48.968	1.00	40.04	A
ATOM	421	O	PHE	A	55	48.120	9.706	48.316	1.00	43.34	A
ATOM	422	N	ALA	A	56	50.210	10.351	48.904	1.00	40.28	A
ATOM	423	CA	ALA	A	56	50.169	11.551	48.078	1.00	39.73	A
ATOM	424	CB	ALA	A	56	50.683	12.732	48.873	1.00	34.93	A
ATOM	425	C	ALA	A	56	50.910	11.456	46.746	1.00	39.80	A
ATOM	426	O	ALA	A	56	51.923	10.768	46.613	1.00	39.90	A
ATOM	427	N	MET	A	57	50.370	12.146	45.753	1.00	39.84	A
ATOM	428	CA	MET	A	57	50.974	12.205	44.437	1.00	40.80	A
ATOM	429	CB	MET	A	57	50.090	11.534	43.389	1.00	39.08	A
ATOM	430	CG	MET	A	57	49.830	10.075	43.654	1.00	39.96	A
ATOM	431	SD	MET	A	57	49.830	9.123	42.135	1.00	45.17	A
ATOM	432	CE	MET	A	57	48.384	9.770	41.389	1.00	52.26	A
ATOM	433	C	MET	A	57	51.083	13.695	44.163	1.00	43.85	A
ATOM	434	O	MET	A	57	50.077	14.380	43.948	1.00	41.80	A
ATOM	435	N	LYS	A	58	52.310	14.196	44.200	1.00	47.84	A
ATOM	436	CA	LYS	A	58	52.555	15.608	43.974	1.00	54.71	A
ATOM	437	CB	LYS	A	58	53.646	16.094	44.920	1.00	60.11	A
ATOM	438	CG	LYS	A	58	53.694	17.598	45.085	1.00	67.21	A
ATOM	439	CD	LYS	A	58	54.848	18.011	45.988	1.00	71.96	A
ATOM	440	CE	LYS	A	58	54.593	19.369	46.633	1.00	76.40	A
ATOM	441	NZ	LYS	A	58	53.433	19.316	47.578	1.00	75.23	A
ATOM	442	C	LYS	A	58	52.965	15.879	42.535	1.00	57.17	A
ATOM	443	O	LYS	A	58	53.984	15.372	42.068	1.00	60.73	A
ATOM	444	N	GLY	A	59	52.169	16.683	41.835	1.00	57.99	A
ATOM	445	CA	GLY	A	59	52.479	17.009	40.454	1.00	56.05	A
ATOM	446	C	GLY	A	59	52.534	15.770	39.588	1.00	51.99	A
ATOM	447	O	GLY	A	59	52.151	14.698	40.037	1.00	47.22	A
ATOM	448	N	LYS	A	60	53.011	15.914	38.353	1.00	53.30	A
ATOM	449	CA	LYS	A	60	53.090	14.782	37.435	1.00	56.47	A
ATOM	450	CB	LYS	A	60	53.648	15.213	36.073	1.00	54.61	A
ATOM	451	CG	LYS	A	60	52.831	16.302	35.394	1.00	55.52	A
ATOM	452	CD	LYS	A	60	52.966	16.264	33.883	1.00	60.88	A
ATOM	453	CE	LYS	A	60	52.305	15.019	33.306	1.00	69.72	A
ATOM	454	NZ	LYS	A	60	52.298	14.996	31.812	1.00	76.32	A
ATOM	455	C	LYS	A	60	53.973	13.715	38.049	1.00	56.25	A
ATOM	456	O	LYS	A	60	55.185	13.880	38.144	1.00	58.88	A
ATOM	457	N	LYS	A	61	53.347	12.626	38.475	1.00	51.75	A
ATOM	458	CA	LYS	A	61	54.047	11.521	39.111	1.00	47.89	A
ATOM	459	CB	LYS	A	61	53.939	11.629	40.636	1.00	46.44	A
ATOM	460	CG	LYS	A	61	55.271	11.738	41.355	1.00	54.37	A
ATOM	461	CD	LYS	A	61	55.358	10.753	42.511	1.00	59.29	A
ATOM	462	CE	LYS	A	61	54.288	11.027	43.578	1.00	70.05	A
ATOM	463	NZ	LYS	A	61	54.257	9.991	44.675	1.00	68.00	A
ATOM	464	C	LYS	A	61	53.409	10.217	38.655	1.00	47.76	A
ATOM	465	O	LYS	A	61	52.373	10.215	37.990	1.00	45.68	A
ATOM	466	N	GLU	A	62	54.031	9.105	39.011	1.00	47.60	A
ATOM	467	CA	GLU	A	62	53.503	7.801	38.642	1.00	47.62	A
ATOM	468	CB	GLU	A	62	54.140	7.341	37.336	1.00	50.03	A
ATOM	469	CG	GLU	A	62	53.200	6.560	36.450	1.00	66.86	A
ATOM	470	CD	GLU	A	62	53.442	5.062	36.505	1.00	73.59	A
ATOM	471	OE1	GLU	A	62	53.477	4.498	37.622	1.00	79.17	A
ATOM	472	OE2	GLU	A	62	53.593	4.449	35.424	1.00	74.00	A
ATOM	473	C	GLU	A	62	53.855	6.861	39.787	1.00	44.41	A



ATOM	474	O	GLU	A	62	54.981	6.872	40.276	1.00	49.60	A
ATOM	475	N	ASN	A	63	52.890	6.086	40.255	1.00	39.52	A
ATOM	476	CA	ASN	A	63	53.168	5.176	41.352	1.00	39.57	A
ATOM	477	CB	ASN	A	63	52.705	5.728	42.701	1.00	45.23	A
ATOM	478	CG	ASN	A	63	53.432	6.976	43.104	1.00	50.88	A
ATOM	479	OD1	ASN	A	63	53.007	8.082	42.783	1.00	55.66	A
ATOM	480	ND2	ASN	A	63	54.543	6.811	43.807	1.00	53.75	A
ATOM	481	C	ASN	A	63	52.422	3.914	41.099	1.00	39.45	A
ATOM	482	O	ASN	A	63	51.608	3.847	40.170	1.00	40.86	A
ATOM	483	N	THR	A	64	52.668	2.921	41.946	1.00	36.67	A
ATOM	484	CA	THR	A	64	52.008	1.643	41.789	1.00	36.69	A
ATOM	485	CB	THR	A	64	53.013	0.536	41.545	1.00	34.21	A
ATOM	486	OG1	THR	A	64	53.877	0.908	40.465	1.00	46.99	A
ATOM	487	CG2	THR	A	64	52.291	-0.755	41.206	1.00	30.34	A
ATOM	488	C	THR	A	64	51.144	1.202	42.947	1.00	37.73	A
ATOM	489	O	THR	A	64	51.566	1.223	44.099	1.00	41.52	A
ATOM	490	N	LEU	A	65	49.927	0.795	42.620	1.00	36.85	A
ATOM	491	CA	LEU	A	65	49.000	0.289	43.610	1.00	37.00	A
ATOM	492	CB	LEU	A	65	47.577	0.694	43.250	1.00	32.71	A
ATOM	493	CG	LEU	A	65	47.260	2.179	43.370	1.00	28.50	A
ATOM	494	CD1	LEU	A	65	45.806	2.426	43.080	1.00	24.00	A
ATOM	495	CD2	LEU	A	65	47.589	2.646	44.765	1.00	34.11	A
ATOM	496	C	LEU	A	65	49.130	-1.231	43.571	1.00	39.68	A
ATOM	497	O	LEU	A	65	49.247	-1.805	42.495	1.00	40.31	A
ATOM	498	N	ARG	A	66	49.136	-1.875	44.736	1.00	41.29	A
ATOM	499	CA	ARG	A	66	49.247	-3.328	44.807	1.00	42.44	A
ATOM	500	CB	ARG	A	66	50.493	-3.725	45.598	1.00	46.83	A
ATOM	501	CG	ARG	A	66	51.785	-3.205	44.998	1.00	55.38	A
ATOM	502	CD	ARG	A	66	52.972	-3.452	45.918	1.00	63.92	A
ATOM	503	NE	ARG	A	66	54.080	-2.535	45.647	1.00	65.49	A
ATOM	504	CZ	ARG	A	66	54.820	-2.562	44.545	1.00	64.91	A
ATOM	505	NH1	ARG	A	66	54.573	-3.468	43.609	1.00	67.73	A
ATOM	506	NH2	ARG	A	66	55.795	-1.678	44.375	1.00	66.42	A
ATOM	507	C	ARG	A	66	48.007	-3.884	45.483	1.00	43.47	A
ATOM	508	O	ARG	A	66	47.672	-3.479	46.597	1.00	46.99	A
ATOM	509	N	ILE	A	67	47.322	-4.795	44.798	1.00	40.54	A
ATOM	510	CA	ILE	A	67	46.104	-5.400	45.325	1.00	40.90	A
ATOM	511	CB	ILE	A	67	45.059	-5.653	44.215	1.00	39.11	A
ATOM	512	CG2	ILE	A	67	43.889	-6.423	44.783	1.00	41.97	A
ATOM	513	CG1	ILE	A	67	44.558	-4.336	43.626	1.00	40.04	A
ATOM	514	CD1	ILE	A	67	45.499	-3.707	42.659	1.00	40.41	A
ATOM	515	C	ILE	A	67	46.405	-6.738	46.002	1.00	43.96	A
ATOM	516	O	ILE	A	67	46.889	-7.687	45.371	1.00	45.99	A
ATOM	517	N	LEU	A	68	46.090	-6.819	47.285	1.00	41.33	A
ATOM	518	CA	LEU	A	68	46.349	-8.024	48.036	1.00	41.16	A
ATOM	519	CB	LEU	A	68	46.990	-7.672	49.367	1.00	42.94	A
ATOM	520	CG	LEU	A	68	48.140	-6.685	49.331	1.00	39.91	A
ATOM	521	CD1	LEU	A	68	48.575	-6.431	50.750	1.00	42.26	A
ATOM	522	CD2	LEU	A	68	49.279	-7.241	48.500	1.00	42.74	A
ATOM	523	C	LEU	A	68	45.110	-8.853	48.302	1.00	43.60	A
ATOM	524	O	LEU	A	68	44.056	-8.334	48.684	1.00	38.41	A
ATOM	525	N	ASP	A	69	45.279	-10.159	48.118	1.00	46.41	A
ATOM	526	CA	ASP	A	69	44.240	-11.148	48.324	1.00	45.81	A
ATOM	527	CB	ASP	A	69	44.652	-12.421	47.594	1.00	45.36	A
ATOM	528	CG	ASP	A	69	43.693	-13.568	47.814	1.00	49.76	A
ATOM	529	OD1	ASP	A	69	43.924	-14.639	47.200	1.00	49.67	A
ATOM	530	OD2	ASP	A	69	42.725	-13.409	48.592	1.00	37.19	A
ATOM	531	C	ASP	A	69	44.077	-11.413	49.816	1.00	50.70	A



ATOM	532	O	ASP	A	69	44.955	-11.973	50.451	1.00	55.74	A
ATOM	533	N	ALA	A	70	42.962	-10.996	50.388	1.00	56.46	A
ATOM	534	CA	ALA	A	70	42.732	-11.239	51.803	1.00	63.86	A
ATOM	535	CB	ALA	A	70	42.069	-10.041	52.441	1.00	64.03	A
ATOM	536	C	ALA	A	70	41.829	-12.452	51.918	1.00	71.40	A
ATOM	537	O	ALA	A	70	41.856	-13.178	52.914	1.00	73.20	A
ATOM	538	N	THR	A	71	41.025	-12.664	50.879	1.00	79.04	A
ATOM	539	CA	THR	A	71	40.097	-13.786	50.838	1.00	85.26	A
ATOM	540	CB	THR	A	71	39.150	-13.712	49.604	1.00	82.93	A
ATOM	541	OG1	THR	A	71	38.343	-14.895	49.554	1.00	83.04	A
ATOM	542	CG2	THR	A	71	39.935	-13.586	48.308	1.00	81.32	A
ATOM	543	C	THR	A	71	40.843	-15.111	50.817	1.00	91.33	A
ATOM	544	O	THR	A	71	41.361	-15.532	49.775	1.00	92.62	A
ATOM	545	N	ASN	A	72	40.901	-15.755	51.980	1.00	95.07	A
ATOM	546	CA	ASN	A	72	41.577	-17.039	52.114	1.00	99.70	A
ATOM	547	CB	ASN	A	72	41.623	-17.458	53.590	1.00	104.68	A
ATOM	548	CG	ASN	A	72	42.720	-16.746	54.370	1.00	108.97	A
ATOM	549	OD1	ASN	A	72	42.890	-16.974	55.573	1.00	109.76	A
ATOM	550	ND2	ASN	A	72	43.478	-15.886	53.687	1.00	109.90	A
ATOM	551	C	ASN	A	72	40.888	-18.127	51.286	1.00	100.06	A
ATOM	552	O	ASN	A	72	40.287	-19.053	51.836	1.00	101.61	A
ATOM	553	N	ASN	A	73	40.976	-18.008	49.964	1.00	98.34	A
ATOM	554	CA	ASN	A	73	40.365	-18.977	49.058	1.00	95.26	A
ATOM	555	CB	ASN	A	73	41.224	-20.247	48.985	1.00	97.32	A
ATOM	556	CG	ASN	A	73	42.714	-19.949	48.919	1.00	98.90	A
ATOM	557	OD1	ASN	A	73	43.299	-19.417	49.866	1.00	99.05	A
ATOM	558	ND2	ASN	A	73	43.336	-20.296	47.799	1.00	97.95	A
ATOM	559	C	ASN	A	73	38.955	-19.346	49.535	1.00	91.54	A
ATOM	560	O	ASN	A	73	38.537	-20.499	49.424	1.00	91.21	A
ATOM	561	N	GLN	A	74	38.233	-18.366	50.074	1.00	85.54	A
ATOM	562	CA	GLN	A	74	36.877	-18.592	50.570	1.00	80.08	A
ATOM	563	CB	GLN	A	74	36.630	-17.724	51.813	1.00	86.66	A
ATOM	564	CG	GLN	A	74	37.586	-18.045	52.980	1.00	95.33	A
ATOM	565	CD	GLN	A	74	37.648	-16.953	54.059	1.00	98.36	A
ATOM	566	OE1	GLN	A	74	38.367	-17.091	55.055	1.00	96.31	A
ATOM	567	NE2	GLN	A	74	36.902	-15.868	53.858	1.00	97.60	A
ATOM	568	C	GLN	A	74	35.855	-18.267	49.485	1.00	72.34	A
ATOM	569	O	GLN	A	74	34.654	-18.165	49.751	1.00	70.12	A
ATOM	570	N	LEU	A	75	36.348	-18.110	48.258	1.00	63.12	A
ATOM	571	CA	LEU	A	75	35.503	-17.789	47.112	1.00	58.03	A
ATOM	572	CB	LEU	A	75	36.149	-16.687	46.263	1.00	48.34	A
ATOM	573	CG	LEU	A	75	36.387	-15.313	46.882	1.00	41.97	A
ATOM	574	CD1	LEU	A	75	37.344	-14.547	46.017	1.00	33.36	A
ATOM	575	CD2	LEU	A	75	35.077	-14.567	47.043	1.00	39.69	A
ATOM	576	C	LEU	A	75	35.297	-19.007	46.228	1.00	58.98	A
ATOM	577	O	LEU	A	75	36.066	-19.962	46.282	1.00	61.87	A
ATOM	578	N	PRO	A	76	34.247	-18.990	45.399	1.00	57.76	A
ATOM	579	CD	PRO	A	76	33.179	-17.981	45.323	1.00	59.33	A
ATOM	580	CA	PRO	A	76	33.968	-20.109	44.497	1.00	59.21	A
ATOM	581	CB	PRO	A	76	32.805	-19.584	43.663	1.00	55.89	A
ATOM	582	CG	PRO	A	76	32.069	-18.744	44.630	1.00	54.17	A
ATOM	583	C	PRO	A	76	35.216	-20.381	43.645	1.00	62.11	A
ATOM	584	O	PRO	A	76	35.864	-19.438	43.192	1.00	61.27	A
ATOM	585	N	GLN	A	77	35.545	-21.655	43.423	1.00	64.43	A
ATOM	586	CA	GLN	A	77	36.729	-22.004	42.641	1.00	65.67	A
ATOM	587	CB	GLN	A	77	37.551	-23.050	43.391	1.00	66.33	A
ATOM	588	CG	GLN	A	77	38.102	-22.528	44.697	1.00	70.54	A
ATOM	589	CD	GLN	A	77	38.920	-21.269	44.504	1.00	74.29	A



ATOM	590	OE1	GLN	A	77	38.746	-20.279	45.225	1.00	72.21	A
ATOM	591	NE2	GLN	A	77	39.826	-21.299	43.529	1.00	74.12	A
ATOM	592	C	GLN	A	77	36.473	-22.480	41.210	1.00	64.93	A
ATOM	593	O	GLN	A	77	37.412	-22.800	40.482	1.00	64.36	A
ATOM	594	N	ASP	A	78	35.209	-22.501	40.804	1.00	62.06	A
ATOM	595	CA	ASP	A	78	34.850	-22.936	39.463	1.00	59.81	A
ATOM	596	CB	ASP	A	78	33.600	-23.819	39.522	1.00	60.16	A
ATOM	597	CG	ASP	A	78	32.422	-23.128	40.186	1.00	64.25	A
ATOM	598	OD1	ASP	A	78	31.281	-23.598	40.011	1.00	67.41	A
ATOM	599	OD2	ASP	A	78	32.624	-22.122	40.894	1.00	68.85	A
ATOM	600	C	ASP	A	78	34.596	-21.773	38.504	1.00	60.48	A
ATOM	601	O	ASP	A	78	34.555	-21.954	37.284	1.00	61.48	A
ATOM	602	N	ARG	A	79	34.441	-20.574	39.053	1.00	59.75	A
ATOM	603	CA	ARG	A	79	34.144	-19.401	38.239	1.00	53.65	A
ATOM	604	CB	ARG	A	79	32.637	-19.186	38.221	1.00	53.59	A
ATOM	605	CG	ARG	A	79	32.068	-18.866	39.599	1.00	53.65	A
ATOM	606	CD	ARG	A	79	30.580	-19.089	39.651	1.00	53.10	A
ATOM	607	NE	ARG	A	79	30.298	-20.515	39.592	1.00	59.91	A
ATOM	608	CZ	ARG	A	79	29.096	-21.040	39.393	1.00	59.96	A
ATOM	609	NH1	ARG	A	79	28.036	-20.255	39.230	1.00	56.86	A
ATOM	610	NH2	ARG	A	79	28.962	-22.360	39.346	1.00	60.89	A
ATOM	611	C	ARG	A	79	34.803	-18.175	38.819	1.00	48.41	A
ATOM	612	O	ARG	A	79	35.309	-18.212	39.935	1.00	49.07	A
ATOM	613	N	GLU	A	80	34.789	-17.085	38.062	1.00	45.30	A
ATOM	614	CA	GLU	A	80	35.366	-15.835	38.540	1.00	41.81	A
ATOM	615	CB	GLU	A	80	35.597	-14.850	37.405	1.00	38.87	A
ATOM	616	CG	GLU	A	80	36.423	-15.323	36.244	1.00	35.20	A
ATOM	617	CD	GLU	A	80	36.578	-14.225	35.208	1.00	36.07	A
ATOM	618	OE1	GLU	A	80	37.711	-13.744	35.000	1.00	31.43	A
ATOM	619	OE2	GLU	A	80	35.554	-13.828	34.607	1.00	42.76	A
ATOM	620	C	GLU	A	80	34.357	-15.190	39.483	1.00	42.83	A
ATOM	621	O	GLU	A	80	33.152	-15.440	39.393	1.00	42.30	A
ATOM	622	N	SER	A	81	34.849	-14.358	40.390	1.00	41.48	A
ATOM	623	CA	SER	A	81	33.965	-13.659	41.303	1.00	40.00	A
ATOM	624	CB	SER	A	81	34.345	-13.954	42.751	1.00	39.78	A
ATOM	625	OG	SER	A	81	34.223	-15.341	43.031	1.00	46.97	A
ATOM	626	C	SER	A	81	34.145	-12.188	40.971	1.00	40.53	A
ATOM	627	O	SER	A	81	35.274	-11.724	40.785	1.00	42.69	A
ATOM	628	N	LEU	A	82	33.037	-11.462	40.861	1.00	38.09	A
ATOM	629	CA	LEU	A	82	33.090	-10.045	40.525	1.00	35.91	A
ATOM	630	CB	LEU	A	82	31.792	-9.624	39.838	1.00	33.68	A
ATOM	631	CG	LEU	A	82	31.520	-8.125	39.671	1.00	34.53	A
ATOM	632	CD1	LEU	A	82	32.701	-7.380	39.073	1.00	30.29	A
ATOM	633	CD2	LEU	A	82	30.310	-7.977	38.795	1.00	37.24	A
ATOM	634	C	LEU	A	82	33.342	-9.137	41.719	1.00	36.58	A
ATOM	635	O	LEU	A	82	32.706	-9.282	42.774	1.00	35.63	A
ATOM	636	N	PHE	A	83	34.282	-8.207	41.543	1.00	34.28	A
ATOM	637	CA	PHE	A	83	34.623	-7.230	42.574	1.00	32.45	A
ATOM	638	CB	PHE	A	83	35.901	-7.616	43.303	1.00	32.53	A
ATOM	639	CG	PHE	A	83	35.726	-8.743	44.272	1.00	39.34	A
ATOM	640	CD1	PHE	A	83	35.694	-10.065	43.835	1.00	28.36	A
ATOM	641	CD2	PHE	A	83	35.546	-8.476	45.634	1.00	41.26	A
ATOM	642	CE1	PHE	A	83	35.482	-11.094	44.734	1.00	28.53	A
ATOM	643	CE2	PHE	A	83	35.334	-9.507	46.540	1.00	33.52	A
ATOM	644	CZ	PHE	A	83	35.303	-10.818	46.082	1.00	34.96	A
ATOM	645	C	PHE	A	83	34.825	-5.872	41.928	1.00	34.82	A
ATOM	646	O	PHE	A	83	34.972	-5.773	40.714	1.00	38.70	A
ATOM	647	N	TRP	A	84	34.829	-4.819	42.738	1.00	33.41	A



ATOM	648	CA	TRP	A	84	35.025	-3.488	42.210	1.00	26.69	A
ATOM	649	CB	TRP	A	84	33.738	-2.684	42.291	1.00	19.98	A
ATOM	650	CG	TRP	A	84	32.670	-3.249	41.424	1.00	22.79	A
ATOM	651	CD2	TRP	A	84	32.433	-2.955	40.037	1.00	16.75	A
ATOM	652	CE2	TRP	A	84	31.334	-3.733	39.626	1.00	19.29	A
ATOM	653	CE3	TRP	A	84	33.045	-2.113	39.104	1.00	21.89	A
ATOM	654	CD1	TRP	A	84	31.738	-4.169	41.781	1.00	22.67	A
ATOM	655	NE1	TRP	A	84	30.925	-4.464	40.710	1.00	24.57	A
ATOM	656	CZ2	TRP	A	84	30.831	-3.696	38.319	1.00	15.65	A
ATOM	657	CZ3	TRP	A	84	32.546	-2.075	37.807	1.00	14.23	A
ATOM	658	CH2	TRP	A	84	31.450	-2.861	37.430	1.00	16.41	A
ATOM	659	C	TRP	A	84	36.145	-2.755	42.904	1.00	31.00	A
ATOM	660	O	TRP	A	84	36.158	-2.608	44.124	1.00	34.22	A
ATOM	661	N	MET	A	85	37.085	-2.302	42.080	1.00	32.40	A
ATOM	662	CA	MET	A	85	38.274	-1.578	42.484	1.00	28.99	A
ATOM	663	CB	MET	A	85	39.413	-2.006	41.544	1.00	28.25	A
ATOM	664	CG	MET	A	85	40.702	-1.212	41.645	1.00	31.75	A
ATOM	665	SD	MET	A	85	41.655	-1.626	43.077	1.00	42.03	A
ATOM	666	CE	MET	A	85	43.040	-0.483	42.930	1.00	36.39	A
ATOM	667	C	MET	A	85	37.979	-0.073	42.377	1.00	29.76	A
ATOM	668	O	MET	A	85	37.517	0.415	41.332	1.00	28.56	A
ATOM	669	N	ASN	A	86	38.239	0.653	43.463	1.00	29.89	A
ATOM	670	CA	ASN	A	86	37.997	2.098	43.517	1.00	26.75	A
ATOM	671	CB	ASN	A	86	36.858	2.423	44.517	1.00	21.46	A
ATOM	672	CG	ASN	A	86	35.492	1.851	44.086	1.00	31.16	A
ATOM	673	OD1	ASN	A	86	35.202	0.661	44.282	1.00	29.74	A
ATOM	674	ND2	ASN	A	86	34.652	2.700	43.499	1.00	22.01	A
ATOM	675	C	ASN	A	86	39.261	2.864	43.917	1.00	26.10	A
ATOM	676	O	ASN	A	86	39.937	2.505	44.874	1.00	28.65	A
ATOM	677	N	VAL	A	87	39.566	3.925	43.181	1.00	26.23	A
ATOM	678	CA	VAL	A	87	40.737	4.759	43.442	1.00	21.94	A
ATOM	679	CB	VAL	A	87	41.826	4.557	42.354	1.00	19.79	A
ATOM	680	CG1	VAL	A	87	43.008	5.474	42.597	1.00	12.81	A
ATOM	681	CG2	VAL	A	87	42.291	3.096	42.359	1.00	14.72	A
ATOM	682	C	VAL	A	87	40.222	6.191	43.422	1.00	26.19	A
ATOM	683	O	VAL	A	87	39.786	6.717	42.390	1.00	24.87	A
ATOM	684	N	LYS	A	88	40.262	6.793	44.601	1.00	28.16	A
ATOM	685	CA	LYS	A	88	39.788	8.141	44.835	1.00	29.76	A
ATOM	686	CB	LYS	A	88	39.054	8.161	46.161	1.00	27.08	A
ATOM	687	CG	LYS	A	88	38.589	9.496	46.637	1.00	31.38	A
ATOM	688	CD	LYS	A	88	37.484	9.265	47.639	1.00	35.87	A
ATOM	689	CE	LYS	A	88	37.282	10.433	48.557	1.00	34.72	A
ATOM	690	NZ	LYS	A	88	36.337	10.007	49.613	1.00	43.74	A
ATOM	691	C	LYS	A	88	40.919	9.139	44.863	1.00	32.40	A
ATOM	692	O	LYS	A	88	41.959	8.868	45.444	1.00	40.28	A
ATOM	693	N	ALA	A	89	40.720	10.290	44.232	1.00	32.42	A
ATOM	694	CA	ALA	A	89	41.741	11.326	44.216	1.00	35.15	A
ATOM	695	CB	ALA	A	89	41.989	11.806	42.791	1.00	38.69	A
ATOM	696	C	ALA	A	89	41.262	12.477	45.085	1.00	36.67	A
ATOM	697	O	ALA	A	89	40.396	13.257	44.693	1.00	36.27	A
ATOM	698	N	ILE	A	90	41.830	12.574	46.275	1.00	38.86	A
ATOM	699	CA	ILE	A	90	41.450	13.623	47.205	1.00	45.38	A
ATOM	700	CB	ILE	A	90	41.622	13.153	48.663	1.00	44.30	A
ATOM	701	CG2	ILE	A	90	41.294	14.295	49.609	1.00	40.12	A
ATOM	702	CG1	ILE	A	90	40.726	11.943	48.935	1.00	41.90	A
ATOM	703	CD1	ILE	A	90	40.923	11.323	50.303	1.00	40.34	A
ATOM	704	C	ILE	A	90	42.269	14.903	47.019	1.00	49.98	A
ATOM	705	O	ILE	A	90	43.500	14.905	47.160	1.00	52.68	A



ATOM	706	N	PRO	A	91	41.597	16.013	46.699	1.00	51.11	A
ATOM	707	CD	PRO	A	91	40.180	16.218	46.373	1.00	51.05	A
ATOM	708	CA	PRO	A	91	42.354	17.247	46.525	1.00	54.88	A
ATOM	709	CB	PRO	A	91	41.354	18.160	45.836	1.00	49.07	A
ATOM	710	CG	PRO	A	91	40.073	17.721	46.406	1.00	51.93	A
ATOM	711	C	PRO	A	91	42.805	17.764	47.888	1.00	60.33	A
ATOM	712	O	PRO	A	91	43.021	16.988	48.812	1.00	62.83	A
ATOM	713	N	SER	A	92	42.951	19.073	48.011	1.00	66.52	A
ATOM	714	CA	SER	A	92	43.388	19.674	49.260	1.00	69.61	A
ATOM	715	CB	SER	A	92	44.878	19.989	49.162	1.00	68.06	A
ATOM	716	OG	SER	A	92	45.211	20.344	47.826	1.00	67.26	A
ATOM	717	C	SER	A	92	42.574	20.935	49.474	1.00	73.36	A
ATOM	718	O	SER	A	92	42.171	21.568	48.506	1.00	74.49	A
ATOM	719	N	MET	A	93	42.329	21.300	50.731	1.00	79.16	A
ATOM	720	CA	MET	A	93	41.530	22.489	51.042	1.00	84.90	A
ATOM	721	CB	MET	A	93	41.031	22.432	52.498	1.00	90.19	A
ATOM	722	CG	MET	A	93	39.860	23.381	52.826	1.00	98.95	A
ATOM	723	SD	MET	A	93	40.266	25.089	53.357	1.00	107.65	A
ATOM	724	CE	MET	A	93	39.575	25.104	55.016	1.00	102.52	A
ATOM	725	C	MET	A	93	42.289	23.792	50.816	1.00	86.06	A
ATOM	726	O	MET	A	93	43.365	23.993	51.380	1.00	85.06	A
ATOM	727	N	ASP	A	94	41.730	24.668	49.978	1.00	88.61	A
ATOM	728	CA	ASP	A	94	42.347	25.963	49.708	1.00	90.81	A
ATOM	729	CB	ASP	A	94	41.677	26.698	48.535	1.00	92.84	A
ATOM	730	CG	ASP	A	94	41.750	25.936	47.221	1.00	96.92	A
ATOM	731	OD1	ASP	A	94	41.812	26.599	46.158	1.00	92.90	A
ATOM	732	OD2	ASP	A	94	41.725	24.686	47.243	1.00	97.61	A
ATOM	733	C	ASP	A	94	42.138	26.810	50.948	1.00	91.50	A
ATOM	734	O	ASP	A	94	41.001	27.036	51.360	1.00	91.94	A
ATOM	735	N	LYS	A	95	43.223	27.269	51.554	1.00	92.54	A
ATOM	736	CA	LYS	A	95	43.099	28.125	52.721	1.00	93.06	A
ATOM	737	CB	LYS	A	95	44.415	28.167	53.496	1.00	92.50	A
ATOM	738	CG	LYS	A	95	44.743	26.875	54.231	1.00	91.52	A
ATOM	739	CD	LYS	A	95	45.179	25.761	53.302	1.00	93.56	A
ATOM	740	CE	LYS	A	95	46.580	26.007	52.754	1.00	93.93	A
ATOM	741	NZ	LYS	A	95	47.085	24.839	51.978	1.00	92.79	A
ATOM	742	C	LYS	A	95	42.771	29.495	52.143	1.00	93.87	A
ATOM	743	O	LYS	A	95	42.622	30.479	52.864	1.00	94.04	A
ATOM	744	N	SER	A	96	42.647	29.520	50.818	1.00	95.24	A
ATOM	745	CA	SER	A	96	42.350	30.724	50.048	1.00	95.48	A
ATOM	746	CB	SER	A	96	43.029	30.629	48.674	1.00	95.68	A
ATOM	747	OG	SER	A	96	42.673	29.431	47.999	1.00	93.18	A
ATOM	748	C	SER	A	96	40.856	31.022	49.854	1.00	94.43	A
ATOM	749	O	SER	A	96	40.456	32.187	49.807	1.00	94.66	A
ATOM	750	N	LYS	A	97	40.037	29.981	49.728	1.00	92.48	A
ATOM	751	CA	LYS	A	97	38.602	30.173	49.532	1.00	90.51	A
ATOM	752	CB	LYS	A	97	38.097	29.292	48.386	1.00	91.65	A
ATOM	753	CG	LYS	A	97	38.961	29.313	47.128	1.00	94.81	A
ATOM	754	CD	LYS	A	97	39.067	30.697	46.514	1.00	99.05	A
ATOM	755	CE	LYS	A	97	39.971	30.677	45.288	1.00	100.93	A
ATOM	756	NZ	LYS	A	97	40.193	32.037	44.722	1.00	102.46	A
ATOM	757	C	LYS	A	97	37.859	29.822	50.814	1.00	87.76	A
ATOM	758	O	LYS	A	97	36.643	29.643	50.813	1.00	87.20	A
ATOM	759	N	LEU	A	98	38.612	29.747	51.904	1.00	86.36	A
ATOM	760	CA	LEU	A	98	38.102	29.402	53.228	1.00	86.15	A
ATOM	761	CB	LEU	A	98	39.235	29.598	54.245	1.00	88.33	A
ATOM	762	CG	LEU	A	98	39.028	29.335	55.739	1.00	89.04	A
ATOM	763	CD1	LEU	A	98	38.376	30.547	56.388	1.00	86.10	A



ATOM	764	CD2	LEU	A	98	38.202	28.066	55.934	1.00	90.05	A
ATOM	765	C	LEU	A	98	36.819	30.107	53.707	1.00	85.13	A
ATOM	766	O	LEU	A	98	35.931	29.456	54.261	1.00	83.73	A
ATOM	767	N	THR	A	99	36.719	31.423	53.510	1.00	84.73	A
ATOM	768	CA	THR	A	99	35.531	32.178	53.939	1.00	81.89	A
ATOM	769	CB	THR	A	99	35.896	33.584	54.480	1.00	83.63	A
ATOM	770	OG1	THR	A	99	36.381	34.399	53.402	1.00	84.87	A
ATOM	771	CG2	THR	A	99	36.965	33.490	55.572	1.00	79.10	A
ATOM	772	C	THR	A	99	34.586	32.365	52.761	1.00	80.15	A
ATOM	773	O	THR	A	99	33.853	33.353	52.676	1.00	78.67	A
ATOM	774	N	GLU	A	100	34.622	31.407	51.845	1.00	79.46	A
ATOM	775	CA	GLU	A	100	33.783	31.443	50.660	1.00	77.45	A
ATOM	776	CB	GLU	A	100	34.651	31.517	49.405	1.00	80.18	A
ATOM	777	CG	GLU	A	100	35.286	32.873	49.165	1.00	87.28	A
ATOM	778	CD	GLU	A	100	36.285	32.850	48.025	1.00	89.03	A
ATOM	779	OE1	GLU	A	100	35.930	32.364	46.929	1.00	91.70	A
ATOM	780	OE2	GLU	A	100	37.424	33.322	48.228	1.00	92.33	A
ATOM	781	C	GLU	A	100	32.888	30.223	50.558	1.00	74.08	A
ATOM	782	O	GLU	A	100	33.115	29.210	51.212	1.00	72.68	A
ATOM	783	N	ASN	A	101	31.856	30.341	49.736	1.00	72.40	A
ATOM	784	CA	ASN	A	101	30.943	29.240	49.499	1.00	69.74	A
ATOM	785	CB	ASN	A	101	29.596	29.774	49.040	1.00	69.70	A
ATOM	786	CG	ASN	A	101	28.633	29.938	50.185	1.00	74.66	A
ATOM	787	OD1	ASN	A	101	29.044	30.097	51.338	1.00	77.59	A
ATOM	788	ND2	ASN	A	101	27.341	29.904	49.882	1.00	74.93	A
ATOM	789	C	ASN	A	101	31.609	28.441	48.404	1.00	67.63	A
ATOM	790	O	ASN	A	101	31.759	28.924	47.280	1.00	67.29	A
ATOM	791	N	THR	A	102	32.020	27.221	48.732	1.00	64.33	A
ATOM	792	CA	THR	A	102	32.724	26.389	47.766	1.00	61.33	A
ATOM	793	CB	THR	A	102	34.200	26.260	48.153	1.00	64.34	A
ATOM	794	OG1	THR	A	102	34.296	25.666	49.453	1.00	70.60	A
ATOM	795	CG2	THR	A	102	34.862	27.628	48.191	1.00	70.03	A
ATOM	796	C	THR	A	102	32.194	24.982	47.556	1.00	56.22	A
ATOM	797	O	THR	A	102	31.444	24.437	48.371	1.00	51.73	A
ATOM	798	N	LEU	A	103	32.592	24.408	46.427	1.00	55.16	A
ATOM	799	CA	LEU	A	103	32.233	23.034	46.079	1.00	52.69	A
ATOM	800	CB	LEU	A	103	31.199	22.952	44.950	1.00	48.23	A
ATOM	801	CG	LEU	A	103	31.022	21.509	44.450	1.00	44.66	A
ATOM	802	CD1	LEU	A	103	30.384	20.669	45.562	1.00	48.29	A
ATOM	803	CD2	LEU	A	103	30.164	21.476	43.206	1.00	47.17	A
ATOM	804	C	LEU	A	103	33.478	22.329	45.595	1.00	49.05	A
ATOM	805	O	LEU	A	103	34.137	22.791	44.666	1.00	47.04	A
ATOM	806	N	GLN	A	104	33.815	21.220	46.233	1.00	48.40	A
ATOM	807	CA	GLN	A	104	34.964	20.465	45.786	1.00	46.05	A
ATOM	808	CB	GLN	A	104	36.010	20.358	46.886	1.00	48.16	A
ATOM	809	CG	GLN	A	104	37.249	21.179	46.567	1.00	49.06	A
ATOM	810	CD	GLN	A	104	38.360	20.990	47.569	1.00	47.06	A
ATOM	811	OE1	GLN	A	104	39.445	21.542	47.410	1.00	49.87	A
ATOM	812	NE2	GLN	A	104	38.099	20.207	48.606	1.00	47.34	A
ATOM	813	C	GLN	A	104	34.540	19.088	45.324	1.00	44.05	A
ATOM	814	O	GLN	A	104	33.649	18.463	45.911	1.00	40.54	A
ATOM	815	N	LEU	A	105	35.163	18.631	44.249	1.00	41.40	A
ATOM	816	CA	LEU	A	105	34.863	17.319	43.729	1.00	39.84	A
ATOM	817	CB	LEU	A	105	34.625	17.383	42.230	1.00	42.67	A
ATOM	818	CG	LEU	A	105	33.441	18.223	41.760	1.00	43.19	A
ATOM	819	CD1	LEU	A	105	33.284	18.046	40.257	1.00	46.81	A
ATOM	820	CD2	LEU	A	105	32.169	17.784	42.467	1.00	49.08	A
ATOM	821	C	LEU	A	105	36.040	16.410	44.007	1.00	37.32	A



ATOM	822	O	LEU	A	105	37.165	16.868	44.135	1.00	42.71	A
ATOM	823	N	ALA	A	106	35.759	15.122	44.132	1.00	33.38	A
ATOM	824	CA	ALA	A	106	36.775	14.107	44.357	1.00	28.96	A
ATOM	825	CB	ALA	A	106	36.627	13.497	45.743	1.00	27.45	A
ATOM	826	C	ALA	A	106	36.506	13.057	43.288	1.00	28.57	A
ATOM	827	O	ALA	A	106	35.505	12.325	43.339	1.00	32.22	A
ATOM	828	N	ILE	A	107	37.382	12.993	42.302	1.00	25.99	A
ATOM	829	CA	ILE	A	107	37.195	12.040	41.228	1.00	23.30	A
ATOM	830	CB	ILE	A	107	38.029	12.413	40.005	1.00	23.35	A
ATOM	831	CG2	ILE	A	107	37.535	11.621	38.791	1.00	22.54	A
ATOM	832	CG1	ILE	A	107	37.903	13.913	39.728	1.00	19.54	A
ATOM	833	CD1	ILE	A	107	36.508	14.350	39.269	1.00	19.67	A
ATOM	834	C	ILE	A	107	37.618	10.670	41.696	1.00	24.89	A
ATOM	835	O	ILE	A	107	38.602	10.528	42.416	1.00	27.65	A
ATOM	836	N	ILE	A	108	36.872	9.658	41.278	1.00	25.44	A
ATOM	837	CA	ILE	A	108	37.174	8.286	41.646	1.00	27.91	A
ATOM	838	CB	ILE	A	108	36.132	7.731	42.647	1.00	29.88	A
ATOM	839	CG2	ILE	A	108	36.515	6.300	43.068	1.00	16.21	A
ATOM	840	CG1	ILE	A	108	36.000	8.694	43.837	1.00	24.38	A
ATOM	841	CD1	ILE	A	108	34.766	8.435	44.690	1.00	17.30	A
ATOM	842	C	ILE	A	108	37.101	7.435	40.391	1.00	28.20	A
ATOM	843	O	ILE	A	108	36.248	7.674	39.528	1.00	26.84	A
ATOM	844	N	SER	A	109	37.996	6.455	40.279	1.00	26.20	A
ATOM	845	CA	SER	A	109	37.956	5.553	39.128	1.00	28.25	A
ATOM	846	CB	SER	A	109	39.331	5.446	38.462	1.00	26.67	A
ATOM	847	OG	SER	A	109	39.790	6.722	38.025	1.00	27.53	A
ATOM	848	C	SER	A	109	37.533	4.230	39.751	1.00	28.09	A
ATOM	849	O	SER	A	109	38.098	3.815	40.767	1.00	31.67	A
ATOM	850	N	ARG	A	110	36.499	3.614	39.188	1.00	21.72	A
ATOM	851	CA	ARG	A	110	35.986	2.349	39.695	1.00	25.62	A
ATOM	852	CB	ARG	A	110	34.548	2.496	40.236	1.00	20.46	A
ATOM	853	CG	ARG	A	110	33.676	1.251	39.989	1.00	24.79	A
ATOM	854	CD	ARG	A	110	32.266	1.319	40.592	1.00	17.11	A
ATOM	855	NE	ARG	A	110	32.356	1.368	42.041	1.00	27.71	A
ATOM	856	CZ	ARG	A	110	31.778	0.515	42.877	1.00	25.45	A
ATOM	857	NH1	ARG	A	110	31.031	-0.485	42.440	1.00	17.47	A
ATOM	858	NH2	ARG	A	110	31.998	0.650	44.171	1.00	26.04	A
ATOM	859	C	ARG	A	110	35.998	1.349	38.544	1.00	32.76	A
ATOM	860	O	ARG	A	110	35.280	1.515	37.544	1.00	30.87	A
ATOM	861	N	ILE	A	111	36.808	0.302	38.699	1.00	33.21	A
ATOM	862	CA	ILE	A	111	36.924	-0.712	37.670	1.00	28.46	A
ATOM	863	CB	ILE	A	111	38.298	-0.643	37.029	1.00	29.44	A
ATOM	864	CG2	ILE	A	111	38.485	0.720	36.372	1.00	25.10	A
ATOM	865	CG1	ILE	A	111	39.370	-0.871	38.089	1.00	29.33	A
ATOM	866	CD1	ILE	A	111	40.768	-0.987	37.513	1.00	29.93	A
ATOM	867	C	ILE	A	111	36.692	-2.123	38.182	1.00	25.36	A
ATOM	868	O	ILE	A	111	36.863	-2.411	39.359	1.00	25.09	A
ATOM	869	N	LYS	A	112	36.305	-3.012	37.283	1.00	23.41	A
ATOM	870	CA	LYS	A	112	36.057	-4.384	37.669	1.00	25.30	A
ATOM	871	CB	LYS	A	112	35.390	-5.143	36.534	1.00	24.01	A
ATOM	872	CG	LYS	A	112	34.244	-4.434	35.880	1.00	22.61	A
ATOM	873	CD	LYS	A	112	33.787	-5.265	34.694	1.00	37.72	A
ATOM	874	CE	LYS	A	112	32.718	-4.579	33.877	1.00	43.07	A
ATOM	875	NZ	LYS	A	112	32.304	-5.437	32.728	1.00	45.86	A
ATOM	876	C	LYS	A	112	37.358	-5.099	38.030	1.00	25.45	A
ATOM	877	O	LYS	A	112	38.413	-4.840	37.470	1.00	27.32	A
ATOM	878	N	LEU	A	113	37.265	-5.995	38.990	1.00	24.01	A
ATOM	879	CA	LEU	A	113	38.393	-6.776	39.423	1.00	27.44	A



ATOM	880	CB	LEU	A	113	38.843	-6.338	40.816	1.00	25.61	A
ATOM	881	CG	LEU	A	113	39.787	-7.285	41.562	1.00	31.16	A
ATOM	882	CD1	LEU	A	113	40.778	-7.900	40.602	1.00	43.08	A
ATOM	883	CD2	LEU	A	113	40.536	-6.515	42.622	1.00	33.73	A
ATOM	884	C	LEU	A	113	37.847	-8.194	39.462	1.00	32.46	A
ATOM	885	O	LEU	A	113	36.899	-8.465	40.199	1.00	39.58	A
ATOM	886	N	TYR	A	114	38.396	-9.091	38.644	1.00	28.70	A
ATOM	887	CA	TYR	A	114	37.911	-10.460	38.670	1.00	29.42	A
ATOM	888	CB	TYR	A	114	37.707	-11.032	37.265	1.00	27.75	A
ATOM	889	CG	TYR	A	114	36.707	-10.315	36.409	1.00	27.87	A
ATOM	890	CD1	TYR	A	114	37.122	-9.570	35.308	1.00	23.04	A
ATOM	891	CE1	TYR	A	114	36.216	-8.902	34.522	1.00	24.87	A
ATOM	892	CD2	TYR	A	114	35.346	-10.373	36.696	1.00	28.15	A
ATOM	893	CE2	TYR	A	114	34.421	-9.709	35.907	1.00	29.56	A
ATOM	894	CZ	TYR	A	114	34.863	-8.975	34.822	1.00	30.53	A
ATOM	895	OH	TYR	A	114	33.950	-8.327	34.023	1.00	35.32	A
ATOM	896	C	TYR	A	114	38.886	-11.362	39.398	1.00	35.05	A
ATOM	897	O	TYR	A	114	40.106	-11.296	39.195	1.00	35.23	A
ATOM	898	N	TYR	A	115	38.337	-12.196	40.265	1.00	37.76	A
ATOM	899	CA	TYR	A	115	39.129	-13.173	40.978	1.00	41.52	A
ATOM	900	CB	TYR	A	115	38.482	-13.488	42.319	1.00	41.85	A
ATOM	901	CG	TYR	A	115	39.186	-14.568	43.086	1.00	46.23	A
ATOM	902	CD1	TYR	A	115	40.413	-14.321	43.701	1.00	49.81	A
ATOM	903	CE1	TYR	A	115	41.071	-15.309	44.420	1.00	50.09	A
ATOM	904	CD2	TYR	A	115	38.630	-15.843	43.205	1.00	47.04	A
ATOM	905	CE2	TYR	A	115	39.282	-16.844	43.924	1.00	48.48	A
ATOM	906	CZ	TYR	A	115	40.503	-16.568	44.529	1.00	51.49	A
ATOM	907	OH	TYR	A	115	41.163	-17.544	45.242	1.00	57.64	A
ATOM	908	C	TYR	A	115	38.970	-14.359	40.034	1.00	44.16	A
ATOM	909	O	TYR	A	115	37.873	-14.891	39.897	1.00	48.01	A
ATOM	910	N	ARG	A	116	40.038	-14.753	39.353	1.00	49.13	A
ATOM	911	CA	ARG	A	116	39.951	-15.865	38.414	1.00	49.36	A
ATOM	912	CB	ARG	A	116	40.607	-15.480	37.091	1.00	52.51	A
ATOM	913	CG	ARG	A	116	40.571	-16.578	36.030	1.00	55.08	A
ATOM	914	CD	ARG	A	116	41.012	-16.040	34.680	1.00	48.05	A
ATOM	915	NE	ARG	A	116	40.032	-15.103	34.156	1.00	50.54	A
ATOM	916	CZ	ARG	A	116	40.300	-14.175	33.247	1.00	48.06	A
ATOM	917	NH1	ARG	A	116	41.529	-14.064	32.767	1.00	47.83	A
ATOM	918	NH2	ARG	A	116	39.339	-13.366	32.813	1.00	42.20	A
ATOM	919	C	ARG	A	116	40.602	-17.119	38.955	1.00	51.49	A
ATOM	920	O	ARG	A	116	41.820	-17.234	38.963	1.00	52.86	A
ATOM	921	N	PRO	A	117	39.792	-18.078	39.421	1.00	56.20	A
ATOM	922	CD	PRO	A	117	38.320	-18.103	39.413	1.00	58.20	A
ATOM	923	CA	PRO	A	117	40.327	-19.329	39.961	1.00	62.62	A
ATOM	924	CB	PRO	A	117	39.082	-20.198	40.121	1.00	60.18	A
ATOM	925	CG	PRO	A	117	38.018	-19.206	40.397	1.00	57.51	A
ATOM	926	C	PRO	A	117	41.287	-19.912	38.946	1.00	67.46	A
ATOM	927	O	PRO	A	117	40.859	-20.413	37.916	1.00	72.30	A
ATOM	928	N	ALA	A	118	42.579	-19.826	39.217	1.00	72.91	A
ATOM	929	CA	ALA	A	118	43.567	-20.356	38.290	1.00	78.78	A
ATOM	930	CB	ALA	A	118	44.973	-19.869	38.686	1.00	82.85	A
ATOM	931	C	ALA	A	118	43.498	-21.881	38.322	1.00	79.93	A
ATOM	932	O	ALA	A	118	44.168	-22.511	39.139	1.00	81.34	A
ATOM	933	N	LYS	A	119	42.686	-22.461	37.434	1.00	80.10	A
ATOM	934	CA	LYS	A	119	42.508	-23.913	37.360	1.00	80.33	A
ATOM	935	CB	LYS	A	119	42.280	-24.483	38.763	1.00	82.51	A
ATOM	936	CG	LYS	A	119	42.575	-25.970	38.913	1.00	85.21	A
ATOM	937	CD	LYS	A	119	44.069	-26.242	39.056	1.00	85.87	A



ATOM	938	CE	LYS	A	119	44.322	-27.673	39.537	1.00	89.17	A
ATOM	939	NZ	LYS	A	119	45.753	-27.955	39.856	1.00	91.51	A
ATOM	940	C	LYS	A	119	41.301	-24.267	36.482	1.00	79.96	A
ATOM	941	O	LYS	A	119	40.769	-25.380	36.556	1.00	79.84	A
ATOM	942	N	LEU	A	120	40.874	-23.323	35.650	1.00	78.20	A
ATOM	943	CA	LEU	A	120	39.717	-23.538	34.786	1.00	76.07	A
ATOM	944	CB	LEU	A	120	38.958	-22.223	34.611	1.00	76.08	A
ATOM	945	CG	LEU	A	120	38.762	-21.423	35.904	1.00	73.67	A
ATOM	946	CD1	LEU	A	120	38.028	-20.130	35.600	1.00	73.40	A
ATOM	947	CD2	LEU	A	120	37.997	-22.251	36.922	1.00	72.60	A
ATOM	948	C	LEU	A	120	40.116	-24.094	33.426	1.00	74.76	A
ATOM	949	O	LEU	A	120	41.206	-23.817	32.923	1.00	75.67	A
ATOM	950	N	ALA	A	121	39.219	-24.875	32.832	1.00	73.89	A
ATOM	951	CA	ALA	A	121	39.476	-25.495	31.534	1.00	72.13	A
ATOM	952	CB	ALA	A	121	38.502	-26.645	31.312	1.00	70.99	A
ATOM	953	C	ALA	A	121	39.383	-24.512	30.378	1.00	69.72	A
ATOM	954	O	ALA	A	121	40.385	-24.140	29.776	1.00	68.65	A
ATOM	955	N	LEU	A	122	38.166	-24.099	30.069	1.00	69.24	A
ATOM	956	CA	LEU	A	122	37.938	-23.172	28.980	1.00	70.03	A
ATOM	957	CB	LEU	A	122	36.458	-22.799	28.934	1.00	66.75	A
ATOM	958	CG	LEU	A	122	36.054	-21.628	28.039	1.00	67.55	A
ATOM	959	CD1	LEU	A	122	36.852	-21.649	26.746	1.00	64.99	A
ATOM	960	CD2	LEU	A	122	34.553	-21.701	27.779	1.00	66.80	A
ATOM	961	C	LEU	A	122	38.788	-21.914	29.084	1.00	72.04	A
ATOM	962	O	LEU	A	122	38.558	-21.076	29.946	1.00	74.93	A
ATOM	963	N	PRO	A	123	39.780	-21.760	28.195	1.00	72.72	A
ATOM	964	CD	PRO	A	123	40.142	-22.671	27.094	1.00	73.51	A
ATOM	965	CA	PRO	A	123	40.653	-20.579	28.212	1.00	73.02	A
ATOM	966	CB	PRO	A	123	41.753	-20.962	27.226	1.00	74.93	A
ATOM	967	CG	PRO	A	123	41.006	-21.783	26.211	1.00	75.79	A
ATOM	968	C	PRO	A	123	39.899	-19.299	27.803	1.00	70.69	A
ATOM	969	O	PRO	A	123	39.200	-19.271	26.786	1.00	70.37	A
ATOM	970	N	PRO	A	124	40.054	-18.221	28.588	1.00	67.18	A
ATOM	971	CD	PRO	A	124	41.089	-18.106	29.624	1.00	65.62	A
ATOM	972	CA	PRO	A	124	39.411	-16.921	28.366	1.00	64.43	A
ATOM	973	CB	PRO	A	124	40.301	-15.947	29.146	1.00	61.21	A
ATOM	974	CG	PRO	A	124	41.563	-16.713	29.405	1.00	65.82	A
ATOM	975	C	PRO	A	124	39.198	-16.499	26.918	1.00	65.52	A
ATOM	976	O	PRO	A	124	38.151	-15.956	26.569	1.00	64.73	A
ATOM	977	N	ASP	A	125	40.185	-16.742	26.074	1.00	68.42	A
ATOM	978	CA	ASP	A	125	40.078	-16.388	24.663	1.00	72.75	A
ATOM	979	CB	ASP	A	125	41.328	-16.857	23.946	1.00	79.90	A
ATOM	980	CG	ASP	A	125	41.606	-18.324	24.204	1.00	88.64	A
ATOM	981	OD1	ASP	A	125	40.853	-19.188	23.696	1.00	89.36	A
ATOM	982	OD2	ASP	A	125	42.568	-18.616	24.941	1.00	95.14	A
ATOM	983	C	ASP	A	125	38.878	-17.081	24.024	1.00	73.33	A
ATOM	984	O	ASP	A	125	38.199	-16.526	23.160	1.00	72.46	A
ATOM	985	N	GLN	A	126	38.635	-18.306	24.471	1.00	73.82	A
ATOM	986	CA	GLN	A	126	37.574	-19.158	23.957	1.00	76.31	A
ATOM	987	CB	GLN	A	126	38.101	-20.604	24.013	1.00	82.74	A
ATOM	988	CG	GLN	A	126	37.267	-21.713	23.362	1.00	87.98	A
ATOM	989	CD	GLN	A	126	37.961	-23.078	23.462	1.00	89.86	A
ATOM	990	OE1	GLN	A	126	37.348	-24.128	23.237	1.00	89.72	A
ATOM	991	NE2	GLN	A	126	39.250	-23.060	23.799	1.00	87.56	A
ATOM	992	C	GLN	A	126	36.239	-19.017	24.709	1.00	75.96	A
ATOM	993	O	GLN	A	126	35.495	-19.989	24.846	1.00	78.10	A
ATOM	994	N	ALA	A	127	35.919	-17.810	25.175	1.00	73.07	A
ATOM	995	CA	ALA	A	127	34.676	-17.602	25.925	1.00	68.39	A



ATOM	996	CB	ALA	A	127	34.981	-16.896	27.235	1.00	60.93	A
ATOM	997	C	ALA	A	127	33.555	-16.865	25.184	1.00	66.81	A
ATOM	998	O	ALA	A	127	32.403	-17.283	25.239	1.00	66.02	A
ATOM	999	N	ALA	A	128	33.879	-15.776	24.495	1.00	66.13	A
ATOM	1000	CA	ALA	A	128	32.862	-15.018	23.772	1.00	68.20	A
ATOM	1001	CB	ALA	A	128	33.516	-13.901	22.974	1.00	64.84	A
ATOM	1002	C	ALA	A	128	32.012	-15.896	22.845	1.00	71.74	A
ATOM	1003	O	ALA	A	128	30.793	-15.724	22.764	1.00	71.72	A
ATOM	1004	N	GLU	A	129	32.659	-16.834	22.155	1.00	74.05	A
ATOM	1005	CA	GLU	A	129	31.977	-17.737	21.227	1.00	76.20	A
ATOM	1006	CB	GLU	A	129	32.960	-18.739	20.643	1.00	82.11	A
ATOM	1007	CG	GLU	A	129	34.403	-18.291	20.671	1.00	98.73	A
ATOM	1008	CD	GLU	A	129	35.371	-19.467	20.655	1.00	103.83	A
ATOM	1009	OE1	GLU	A	129	36.590	-19.234	20.466	1.00	106.59	A
ATOM	1010	OE2	GLU	A	129	34.911	-20.621	20.844	1.00	104.99	A
ATOM	1011	C	GLU	A	129	30.875	-18.534	21.909	1.00	76.20	A
ATOM	1012	O	GLU	A	129	29.802	-18.736	21.336	1.00	78.21	A
ATOM	1013	N	LYS	A	130	31.159	-19.006	23.122	1.00	71.91	A
ATOM	1014	CA	LYS	A	130	30.215	-19.813	23.888	1.00	68.25	A
ATOM	1015	CB	LYS	A	130	30.865	-20.291	25.186	1.00	70.75	A
ATOM	1016	CG	LYS	A	130	32.194	-21.020	25.004	1.00	74.67	A
ATOM	1017	CD	LYS	A	130	32.011	-22.386	24.366	1.00	74.27	A
ATOM	1018	CE	LYS	A	130	33.344	-23.059	24.080	1.00	73.75	A
ATOM	1019	NZ	LYS	A	130	33.149	-24.415	23.484	1.00	73.72	A
ATOM	1020	C	LYS	A	130	28.933	-19.071	24.224	1.00	68.00	A
ATOM	1021	O	LYS	A	130	28.026	-19.644	24.827	1.00	67.92	A
ATOM	1022	N	LEU	A	131	28.853	-17.802	23.830	1.00	67.34	A
ATOM	1023	CA	LEU	A	131	27.680	-16.992	24.118	1.00	67.92	A
ATOM	1024	CB	LEU	A	131	28.002	-15.506	23.974	1.00	64.70	A
ATOM	1025	CG	LEU	A	131	26.852	-14.610	24.457	1.00	60.80	A
ATOM	1026	CD1	LEU	A	131	26.757	-14.706	25.984	1.00	54.51	A
ATOM	1027	CD2	LEU	A	131	27.074	-13.177	24.027	1.00	54.96	A
ATOM	1028	C	LEU	A	131	26.484	-17.299	23.242	1.00	72.16	A
ATOM	1029	O	LEU	A	131	26.469	-16.941	22.065	1.00	76.77	A
ATOM	1030	N	ARG	A	132	25.473	-17.939	23.816	1.00	75.27	A
ATOM	1031	CA	ARG	A	132	24.266	-18.262	23.065	1.00	81.32	A
ATOM	1032	CB	ARG	A	132	23.763	-19.650	23.456	1.00	85.77	A
ATOM	1033	CG	ARG	A	132	24.812	-20.748	23.318	1.00	94.11	A
ATOM	1034	CD	ARG	A	132	24.400	-22.004	24.091	1.00	98.71	A
ATOM	1035	NE	ARG	A	132	25.538	-22.878	24.380	1.00	103.00	A
ATOM	1036	CZ	ARG	A	132	25.499	-23.918	25.212	1.00	103.86	A
ATOM	1037	NH1	ARG	A	132	24.374	-24.229	25.847	1.00	101.67	A
ATOM	1038	NH2	ARG	A	132	26.595	-24.639	25.421	1.00	104.18	A
ATOM	1039	C	ARG	A	132	23.201	-17.208	23.368	1.00	82.53	A
ATOM	1040	O	ARG	A	132	23.477	-16.217	24.044	1.00	80.66	A
ATOM	1041	N	PHE	A	133	21.987	-17.414	22.868	1.00	85.49	A
ATOM	1042	CA	PHE	A	133	20.909	-16.460	23.101	1.00	89.99	A
ATOM	1043	CB	PHE	A	133	20.835	-15.460	21.947	1.00	89.83	A
ATOM	1044	CG	PHE	A	133	22.019	-14.545	21.863	1.00	89.92	A
ATOM	1045	CD1	PHE	A	133	23.251	-15.019	21.431	1.00	89.46	A
ATOM	1046	CD2	PHE	A	133	21.907	-13.210	22.242	1.00	90.61	A
ATOM	1047	CE1	PHE	A	133	24.357	-14.180	21.379	1.00	91.51	A
ATOM	1048	CE2	PHE	A	133	23.004	-12.358	22.195	1.00	89.22	A
ATOM	1049	CZ	PHE	A	133	24.234	-12.843	21.762	1.00	90.80	A
ATOM	1050	C	PHE	A	133	19.523	-17.070	23.319	1.00	93.54	A
ATOM	1051	O	PHE	A	133	19.376	-18.258	23.612	1.00	95.64	A
ATOM	1052	N	ARG	A	134	18.512	-16.222	23.177	1.00	95.33	A
ATOM	1053	CA	ARG	A	134	17.110	-16.591	23.342	1.00	98.47	A



ATOM	1054	CB	ARG	A	134	16.836	-17.049	24.770	1.00	96.46	A
ATOM	1055	CG	ARG	A	134	15.363	-17.236	25.084	1.00	96.89	A
ATOM	1056	CD	ARG	A	134	15.143	-17.231	26.586	1.00	99.77	A
ATOM	1057	NE	ARG	A	134	15.884	-18.301	27.247	1.00103.07		A
ATOM	1058	CZ	ARG	A	134	16.197	-18.302	28.539	1.00103.43		A
ATOM	1059	NH1	ARG	A	134	15.836	-17.282	29.312	1.00102.01		A
ATOM	1060	NH2	ARG	A	134	16.869	-19.322	29.061	1.00102.06		A
ATOM	1061	C	ARG	A	134	16.351	-15.303	23.065	1.00101.77		A
ATOM	1062	O	ARG	A	134	16.078	-14.519	23.979	1.00102.68		A
ATOM	1063	N	ARG	A	135	16.006	-15.088	21.799	1.00103.79		A
ATOM	1064	CA	ARG	A	135	15.332	-13.860	21.402	1.00104.26		A
ATOM	1065	CB	ARG	A	135	16.003	-13.313	20.147	1.00104.33		A
ATOM	1066	CG	ARG	A	135	15.770	-14.139	18.904	1.00101.69		A
ATOM	1067	CD	ARG	A	135	14.953	-13.323	17.948	1.00103.33		A
ATOM	1068	NE	ARG	A	135	15.578	-12.021	17.768	1.00102.02		A
ATOM	1069	CZ	ARG	A	135	14.944	-10.940	17.337	1.00103.23		A
ATOM	1070	NH1	ARG	A	135	15.605	-9.799	17.208	1.00103.92		A
ATOM	1071	NH2	ARG	A	135	13.651	-10.997	17.044	1.00103.58		A
ATOM	1072	C	ARG	A	135	13.832	-13.928	21.173	1.00104.63		A
ATOM	1073	O	ARG	A	135	13.367	-14.616	20.267	1.00105.45		A
ATOM	1074	N	SER	A	136	13.081	-13.204	22.000	1.00104.76		A
ATOM	1075	CA	SER	A	136	11.627	-13.140	21.874	1.00106.02		A
ATOM	1076	CB	SER	A	136	10.964	-13.037	23.254	1.00104.91		A
ATOM	1077	OG	SER	A	136	11.050	-14.261	23.963	1.00104.33		A
ATOM	1078	C	SER	A	136	11.301	-11.895	21.045	1.00107.69		A
ATOM	1079	O	SER	A	136	11.995	-11.591	20.071	1.00108.16		A
ATOM	1080	N	ALA	A	137	10.248	-11.179	21.424	1.00107.96		A
ATOM	1081	CA	ALA	A	137	9.859	-9.962	20.719	1.00108.16		A
ATOM	1082	CB	ALA	A	137	8.419	-10.067	20.242	1.00107.11		A
ATOM	1083	C	ALA	A	137	10.008	-8.801	21.695	1.00108.96		A
ATOM	1084	O	ALA	A	137	9.535	-7.688	21.444	1.00109.33		A
ATOM	1085	N	ASN	A	138	10.678	-9.083	22.811	1.00108.20		A
ATOM	1086	CA	ASN	A	138	10.897	-8.099	23.861	1.00106.68		A
ATOM	1087	CB	ASN	A	138	9.569	-7.772	24.554	1.00107.71		A
ATOM	1088	CG	ASN	A	138	8.757	-9.019	24.898	1.00107.21		A
ATOM	1089	OD1	ASN	A	138	9.229	-9.931	25.595	1.00103.20		A
ATOM	1090	ND2	ASN	A	138	7.523	-9.058	24.408	1.00104.18		A
ATOM	1091	C	ASN	A	138	11.904	-8.551	24.912	1.00104.33		A
ATOM	1092	O	ASN	A	138	12.460	-7.729	25.639	1.00102.13		A
ATOM	1093	N	SER	A	139	12.154	-9.853	24.982	1.00103.36		A
ATOM	1094	CA	SER	A	139	13.066	-10.370	25.993	1.00101.80		A
ATOM	1095	CB	SER	A	139	12.255	-11.140	27.041	1.00101.56		A
ATOM	1096	OG	SER	A	139	11.137	-10.379	27.470	1.00102.16		A
ATOM	1097	C	SER	A	139	14.228	-11.241	25.504	1.00100.27		A
ATOM	1098	O	SER	A	139	14.211	-12.464	25.672	1.00100.36		A
ATOM	1099	N	LEU	A	140	15.237	-10.609	24.906	1.00	97.34	A
ATOM	1100	CA	LEU	A	140	16.422	-11.326	24.434	1.00	92.23	A
ATOM	1101	CB	LEU	A	140	17.234	-10.441	23.496	1.00	91.63	A
ATOM	1102	CG	LEU	A	140	18.335	-11.139	22.696	1.00	93.83	A
ATOM	1103	CD1	LEU	A	140	19.083	-10.105	21.856	1.00	92.02	A
ATOM	1104	CD2	LEU	A	140	19.286	-11.863	23.637	1.00	93.87	A
ATOM	1105	C	LEU	A	140	17.246	-11.640	25.683	1.00	89.12	A
ATOM	1106	O	LEU	A	140	17.584	-10.742	26.450	1.00	91.60	A
ATOM	1107	N	THR	A	141	17.590	-12.904	25.880	1.00	84.11	A
ATOM	1108	CA	THR	A	141	18.323	-13.287	27.074	1.00	81.12	A
ATOM	1109	CB	THR	A	141	17.502	-14.328	27.881	1.00	80.24	A
ATOM	1110	OG1	THR	A	141	16.219	-13.770	28.197	1.00	77.38	A
ATOM	1111	CG2	THR	A	141	18.225	-14.717	29.179	1.00	80.24	A



ATOM	1112	C	THR	A	141	19.741	-13.824	26.870	1.00	80.24	A
ATOM	1113	O	THR	A	141	19.933	-15.027	26.658	1.00	79.58	A
ATOM	1114	N	LEU	A	142	20.729	-12.931	26.957	1.00	76.82	A
ATOM	1115	CA	LEU	A	142	22.134	-13.318	26.815	1.00	72.84	A
ATOM	1116	CB	LEU	A	142	23.061	-12.165	27.216	1.00	68.91	A
ATOM	1117	CG	LEU	A	142	23.045	-10.770	26.562	1.00	71.48	A
ATOM	1118	CD1	LEU	A	142	23.732	-10.801	25.214	1.00	66.22	A
ATOM	1119	CD2	LEU	A	142	21.617	-10.252	26.449	1.00	66.28	A
ATOM	1120	C	LEU	A	142	22.357	-14.496	27.766	1.00	71.91	A
ATOM	1121	O	LEU	A	142	21.924	-14.464	28.915	1.00	71.08	A
ATOM	1122	N	ILE	A	143	23.022	-15.538	27.288	1.00	71.51	A
ATOM	1123	CA	ILE	A	143	23.272	-16.709	28.119	1.00	70.41	A
ATOM	1124	CB	ILE	A	143	22.363	-17.881	27.683	1.00	70.24	A
ATOM	1125	CG2	ILE	A	143	22.132	-17.817	26.195	1.00	71.96	A
ATOM	1126	CG1	ILE	A	143	22.972	-19.223	28.096	1.00	69.66	A
ATOM	1127	CD1	ILE	A	143	23.009	-19.457	29.592	1.00	74.41	A
ATOM	1128	C	ILE	A	143	24.733	-17.131	28.063	1.00	70.37	A
ATOM	1129	O	ILE	A	143	25.242	-17.500	27.010	1.00	72.24	A
ATOM	1130	N	ASN	A	144	25.397	-17.076	29.214	1.00	69.73	A
ATOM	1131	CA	ASN	A	144	26.811	-17.429	29.323	1.00	67.88	A
ATOM	1132	CB	ASN	A	144	27.594	-16.225	29.855	1.00	65.44	A
ATOM	1133	CG	ASN	A	144	29.030	-16.559	30.196	1.00	65.15	A
ATOM	1134	OD1	ASN	A	144	29.534	-17.629	29.853	1.00	62.67	A
ATOM	1135	ND2	ASN	A	144	29.706	-15.630	30.868	1.00	63.84	A
ATOM	1136	C	ASN	A	144	27.031	-18.645	30.221	1.00	66.60	A
ATOM	1137	O	ASN	A	144	26.797	-18.591	31.425	1.00	66.49	A
ATOM	1138	N	PRO	A	145	27.482	-19.765	29.631	1.00	66.80	A
ATOM	1139	CD	PRO	A	145	27.470	-19.968	28.167	1.00	67.42	A
ATOM	1140	CA	PRO	A	145	27.752	-21.032	30.321	1.00	65.43	A
ATOM	1141	CB	PRO	A	145	27.378	-22.063	29.274	1.00	64.83	A
ATOM	1142	CG	PRO	A	145	27.924	-21.411	28.025	1.00	67.40	A
ATOM	1143	C	PRO	A	145	29.198	-21.203	30.774	1.00	65.99	A
ATOM	1144	O	PRO	A	145	29.519	-22.140	31.506	1.00	68.84	A
ATOM	1145	N	THR	A	146	30.072	-20.307	30.332	1.00	64.37	A
ATOM	1146	CA	THR	A	146	31.485	-20.374	30.689	1.00	61.20	A
ATOM	1147	CB	THR	A	146	32.296	-19.421	29.813	1.00	60.13	A
ATOM	1148	OG1	THR	A	146	32.406	-18.152	30.461	1.00	48.37	A
ATOM	1149	CG2	THR	A	146	31.598	-19.221	28.472	1.00	58.08	A
ATOM	1150	C	THR	A	146	31.660	-19.958	32.144	1.00	63.71	A
ATOM	1151	O	THR	A	146	30.683	-19.755	32.851	1.00	68.20	A
ATOM	1152	N	PRO	A	147	32.907	-19.850	32.621	1.00	63.27	A
ATOM	1153	CD	PRO	A	147	34.065	-20.642	32.171	1.00	65.51	A
ATOM	1154	CA	PRO	A	147	33.093	-19.440	34.015	1.00	60.71	A
ATOM	1155	CB	PRO	A	147	34.055	-20.482	34.538	1.00	63.94	A
ATOM	1156	CG	PRO	A	147	34.999	-20.596	33.384	1.00	65.82	A
ATOM	1157	C	PRO	A	147	33.679	-18.034	34.114	1.00	58.31	A
ATOM	1158	O	PRO	A	147	34.310	-17.691	35.111	1.00	59.00	A
ATOM	1159	N	TYR	A	148	33.476	-17.230	33.076	1.00	55.78	A
ATOM	1160	CA	TYR	A	148	33.994	-15.860	33.056	1.00	54.68	A
ATOM	1161	CB	TYR	A	148	35.003	-15.657	31.915	1.00	52.42	A
ATOM	1162	CG	TYR	A	148	36.109	-16.669	31.835	1.00	54.53	A
ATOM	1163	CD1	TYR	A	148	35.887	-17.945	31.314	1.00	53.25	A
ATOM	1164	CE1	TYR	A	148	36.916	-18.882	31.249	1.00	52.08	A
ATOM	1165	CD2	TYR	A	148	37.388	-16.355	32.286	1.00	59.18	A
ATOM	1166	CE2	TYR	A	148	38.426	-17.287	32.227	1.00	57.18	A
ATOM	1167	CZ	TYR	A	148	38.182	-18.545	31.712	1.00	56.02	A
ATOM	1168	OH	TYR	A	148	39.205	-19.464	31.703	1.00	60.53	A
ATOM	1169	C	TYR	A	148	32.891	-14.826	32.865	1.00	52.36	A



ATOM	1170	O	TYR	A	148	31.875	-15.091	32.218	1.00	54.15	A
ATOM	1171	N	TYR	A	149	33.096	-13.636	33.412	1.00	46.88	A
ATOM	1172	CA	TYR	A	149	32.109	-12.589	33.232	1.00	45.19	A
ATOM	1173	CB	TYR	A	149	32.338	-11.433	34.219	1.00	43.03	A
ATOM	1174	CG	TYR	A	149	31.664	-11.614	35.559	1.00	42.11	A
ATOM	1175	CD1	TYR	A	149	32.240	-12.391	36.556	1.00	41.82	A
ATOM	1176	CE1	TYR	A	149	31.590	-12.596	37.779	1.00	43.09	A
ATOM	1177	CD2	TYR	A	149	30.420	-11.040	35.814	1.00	45.78	A
ATOM	1178	CE2	TYR	A	149	29.758	-11.242	37.037	1.00	40.20	A
ATOM	1179	CZ	TYR	A	149	30.348	-12.017	38.011	1.00	39.11	A
ATOM	1180	OH	TYR	A	149	29.714	-12.203	39.219	1.00	39.29	A
ATOM	1181	C	TYR	A	149	32.218	-12.086	31.793	1.00	42.46	A
ATOM	1182	O	TYR	A	149	33.292	-11.712	31.333	1.00	43.49	A
ATOM	1183	N	LEU	A	150	31.108	-12.083	31.074	1.00	38.24	A
ATOM	1184	CA	LEU	A	150	31.152	-11.615	29.709	1.00	38.20	A
ATOM	1185	CB	LEU	A	150	30.316	-12.528	28.793	1.00	41.63	A
ATOM	1186	CG	LEU	A	150	30.798	-13.982	28.638	1.00	47.76	A
ATOM	1187	CD1	LEU	A	150	29.923	-14.693	27.628	1.00	49.37	A
ATOM	1188	CD2	LEU	A	150	32.260	-14.027	28.168	1.00	46.98	A
ATOM	1189	C	LEU	A	150	30.658	-10.190	29.624	1.00	37.43	A
ATOM	1190	O	LEU	A	150	29.509	-9.886	29.957	1.00	38.19	A
ATOM	1191	N	THR	A	151	31.538	-9.305	29.186	1.00	37.68	A
ATOM	1192	CA	THR	A	151	31.159	-7.918	29.033	1.00	39.56	A
ATOM	1193	CB	THR	A	151	32.329	-6.956	29.381	1.00	37.50	A
ATOM	1194	OG1	THR	A	151	32.765	-7.189	30.725	1.00	33.72	A
ATOM	1195	CG2	THR	A	151	31.878	-5.504	29.273	1.00	36.25	A
ATOM	1196	C	THR	A	151	30.735	-7.741	27.579	1.00	43.30	A
ATOM	1197	O	THR	A	151	31.529	-7.346	26.726	1.00	45.62	A
ATOM	1198	N	VAL	A	152	29.477	-8.069	27.308	1.00	46.36	A
ATOM	1199	CA	VAL	A	152	28.908	-7.953	25.973	1.00	50.28	A
ATOM	1200	CB	VAL	A	152	27.574	-8.721	25.865	1.00	54.87	A
ATOM	1201	CG1	VAL	A	152	26.896	-8.402	24.544	1.00	53.66	A
ATOM	1202	CG2	VAL	A	152	27.820	-10.218	25.989	1.00	53.64	A
ATOM	1203	C	VAL	A	152	28.635	-6.503	25.633	1.00	51.96	A
ATOM	1204	O	VAL	A	152	27.900	-5.829	26.337	1.00	54.79	A
ATOM	1205	N	THR	A	153	29.232	-6.033	24.548	1.00	55.97	A
ATOM	1206	CA	THR	A	153	29.048	-4.662	24.096	1.00	58.87	A
ATOM	1207	CB	THR	A	153	30.305	-3.816	24.398	1.00	58.83	A
ATOM	1208	OG1	THR	A	153	30.090	-2.452	24.002	1.00	59.83	A
ATOM	1209	CG2	THR	A	153	31.514	-4.391	23.667	1.00	56.99	A
ATOM	1210	C	THR	A	153	28.764	-4.688	22.584	1.00	64.16	A
ATOM	1211	O	THR	A	153	28.926	-5.728	21.927	1.00	63.27	A
ATOM	1212	N	GLU	A	154	28.336	-3.547	22.042	1.00	68.30	A
ATOM	1213	CA	GLU	A	154	27.997	-3.419	20.621	1.00	69.78	A
ATOM	1214	CB	GLU	A	154	29.257	-3.406	19.759	1.00	67.91	A
ATOM	1215	CG	GLU	A	154	30.100	-2.168	19.957	1.00	74.41	A
ATOM	1216	CD	GLU	A	154	31.049	-1.918	18.803	1.00	80.81	A
ATOM	1217	OE1	GLU	A	154	31.805	-0.919	18.846	1.00	81.08	A
ATOM	1218	OE2	GLU	A	154	31.031	-2.721	17.847	1.00	87.45	A
ATOM	1219	C	GLU	A	154	27.064	-4.532	20.161	1.00	70.72	A
ATOM	1220	O	GLU	A	154	27.249	-5.118	19.097	1.00	73.11	A
ATOM	1221	N	LEU	A	155	26.058	-4.816	20.979	1.00	72.02	A
ATOM	1222	CA	LEU	A	155	25.078	-5.850	20.678	1.00	73.50	A
ATOM	1223	CB	LEU	A	155	24.353	-6.279	21.955	1.00	65.70	A
ATOM	1224	CG	LEU	A	155	23.396	-7.462	21.844	1.00	60.65	A
ATOM	1225	CD1	LEU	A	155	24.187	-8.721	21.509	1.00	63.06	A
ATOM	1226	CD2	LEU	A	155	22.649	-7.642	23.149	1.00	58.58	A
ATOM	1227	C	LEU	A	155	24.072	-5.277	19.695	1.00	79.03	A



ATOM	1228	O	LEU	A	155	23.751	-4.091	19.754	1.00	79.45	A
ATOM	1229	N	ASN	A	156	23.573	-6.116	18.793	1.00	85.28	A
ATOM	1230	CA	ASN	A	156	22.603	-5.662	17.804	1.00	88.93	A
ATOM	1231	CB	ASN	A	156	23.339	-5.108	16.594	1.00	87.25	A
ATOM	1232	CG	ASN	A	156	24.418	-4.130	16.988	1.00	89.36	A
ATOM	1233	OD1	ASN	A	156	24.134	-3.059	17.524	1.00	89.06	A
ATOM	1234	ND2	ASN	A	156	25.670	-4.500	16.746	1.00	90.53	A
ATOM	1235	C	ASN	A	156	21.653	-6.765	17.374	1.00	91.63	A
ATOM	1236	O	ASN	A	156	22.066	-7.907	17.158	1.00	89.76	A
ATOM	1237	N	ALA	A	157	20.374	-6.414	17.267	1.00	96.18	A
ATOM	1238	CA	ALA	A	157	19.337	-7.354	16.851	1.00	99.74	A
ATOM	1239	CB	ALA	A	157	17.969	-6.847	17.283	1.00	100.77	A
ATOM	1240	C	ALA	A	157	19.404	-7.455	15.334	1.00	102.40	A
ATOM	1241	O	ALA	A	157	18.387	-7.632	14.659	1.00	103.36	A
ATOM	1242	N	GLY	A	158	20.622	-7.332	14.816	1.00	105.21	A
ATOM	1243	CA	GLY	A	158	20.850	-7.392	13.387	1.00	106.57	A
ATOM	1244	C	GLY	A	158	21.156	-6.006	12.858	1.00	107.97	A
ATOM	1245	O	GLY	A	158	22.228	-5.770	12.299	1.00	108.06	A
ATOM	1246	N	THR	A	159	20.206	-5.093	13.044	1.00	109.17	A
ATOM	1247	CA	THR	A	159	20.343	-3.712	12.592	1.00	111.28	A
ATOM	1248	CB	THR	A	159	19.239	-3.331	11.594	1.00	112.70	A
ATOM	1249	OG1	THR	A	159	17.965	-3.416	12.247	1.00	116.55	A
ATOM	1250	CG2	THR	A	159	19.248	-4.268	10.395	1.00	115.55	A
ATOM	1251	C	THR	A	159	20.196	-2.802	13.795	1.00	111.85	A
ATOM	1252	O	THR	A	159	20.968	-1.860	13.978	1.00	112.27	A
ATOM	1253	N	ARG	A	160	19.187	-3.096	14.608	1.00	112.10	A
ATOM	1254	CA	ARG	A	160	18.912	-2.321	15.804	1.00	113.25	A
ATOM	1255	CB	ARG	A	160	17.617	-2.813	16.458	1.00	118.41	A
ATOM	1256	CG	ARG	A	160	17.133	-1.969	17.637	1.00	125.82	A
ATOM	1257	CD	ARG	A	160	16.451	-0.677	17.169	1.00	131.90	A
ATOM	1258	NE	ARG	A	160	15.752	0.009	18.255	1.00	136.67	A
ATOM	1259	CZ	ARG	A	160	16.332	0.811	19.144	1.00	137.21	A
ATOM	1260	NH1	ARG	A	160	17.637	1.050	19.083	1.00	138.96	A
ATOM	1261	NH2	ARG	A	160	15.606	1.352	20.116	1.00	136.47	A
ATOM	1262	C	ARG	A	160	20.069	-2.472	16.783	1.00	111.18	A
ATOM	1263	O	ARG	A	160	20.605	-3.568	16.967	1.00	110.16	A
ATOM	1264	N	VAL	A	161	20.459	-1.362	17.400	1.00	108.44	A
ATOM	1265	CA	VAL	A	161	21.540	-1.371	18.378	1.00	105.90	A
ATOM	1266	CB	VAL	A	161	22.426	-0.108	18.250	1.00	108.81	A
ATOM	1267	CG1	VAL	A	161	21.584	1.151	18.459	1.00	109.63	A
ATOM	1268	CG2	VAL	A	161	23.573	-0.172	19.255	1.00	107.85	A
ATOM	1269	C	VAL	A	161	20.942	-1.429	19.782	1.00	101.78	A
ATOM	1270	O	VAL	A	161	20.040	-0.658	20.120	1.00	101.40	A
ATOM	1271	N	LEU	A	162	21.445	-2.343	20.602	1.00	97.13	A
ATOM	1272	CA	LEU	A	162	20.930	-2.488	21.957	1.00	93.47	A
ATOM	1273	CB	LEU	A	162	20.695	-3.967	22.263	1.00	93.19	A
ATOM	1274	CG	LEU	A	162	19.669	-4.649	21.364	1.00	92.83	A
ATOM	1275	CD1	LEU	A	162	19.474	-6.093	21.809	1.00	92.94	A
ATOM	1276	CD2	LEU	A	162	18.361	-3.880	21.436	1.00	91.31	A
ATOM	1277	C	LEU	A	162	21.804	-1.878	23.052	1.00	89.80	A
ATOM	1278	O	LEU	A	162	22.695	-1.061	22.795	1.00	88.59	A
ATOM	1279	N	GLU	A	163	21.529	-2.286	24.284	1.00	85.62	A
ATOM	1280	CA	GLU	A	163	22.263	-1.798	25.437	1.00	80.86	A
ATOM	1281	CB	GLU	A	163	21.273	-1.389	26.525	1.00	84.16	A
ATOM	1282	CG	GLU	A	163	21.866	-0.544	27.633	1.00	89.10	A
ATOM	1283	CD	GLU	A	163	20.838	0.383	28.250	1.00	90.24	A
ATOM	1284	OE1	GLU	A	163	20.485	1.389	27.595	1.00	90.20	A
ATOM	1285	OE2	GLU	A	163	20.376	0.102	29.379	1.00	92.14	A



ATOM	1286	C	GLU A 163	23.217	-2.881	25.943	1.00	75.63	A
ATOM	1287	O	GLU A 163	22.847	-4.058	26.051	1.00	74.97	A
ATOM	1288	N	ASN A 164	24.449	-2.469	26.239	1.00	67.82	A
ATOM	1289	CA	ASN A 164	25.494	-3.371	26.715	1.00	60.23	A
ATOM	1290	CB	ASN A 164	26.691	-2.562	27.183	1.00	61.03	A
ATOM	1291	CG	ASN A 164	27.091	-1.509	26.187	1.00	65.34	A
ATOM	1292	OD1	ASN A 164	27.592	-1.816	25.104	1.00	67.49	A
ATOM	1293	ND2	ASN A 164	26.858	-0.251	26.538	1.00	72.33	A
ATOM	1294	C	ASN A 164	25.036	-4.273	27.843	1.00	56.85	A
ATOM	1295	O	ASN A 164	24.095	-3.959	28.564	1.00	60.38	A
ATOM	1296	N	ALA A 165	25.709	-5.399	28.009	1.00	52.80	A
ATOM	1297	CA	ALA A 165	25.332	-6.316	29.065	1.00	51.59	A
ATOM	1298	CB	ALA A 165	24.400	-7.375	28.527	1.00	55.00	A
ATOM	1299	C	ALA A 165	26.550	-6.964	29.682	1.00	52.66	A
ATOM	1300	O	ALA A 165	27.608	-7.063	29.057	1.00	52.84	A
ATOM	1301	N	LEU A 166	26.387	-7.387	30.930	1.00	50.08	A
ATOM	1302	CA	LEU A 166	27.442	-8.042	31.677	1.00	46.09	A
ATOM	1303	CB	LEU A 166	27.784	-7.239	32.930	1.00	39.06	A
ATOM	1304	CG	LEU A 166	28.805	-7.875	33.879	1.00	44.53	A
ATOM	1305	CD1	LEU A 166	30.155	-8.052	33.160	1.00	36.48	A
ATOM	1306	CD2	LEU A 166	28.968	-6.997	35.109	1.00	32.66	A
ATOM	1307	C	LEU A 166	26.849	-9.382	32.050	1.00	45.68	A
ATOM	1308	O	LEU A 166	25.994	-9.467	32.921	1.00	47.46	A
ATOM	1309	N	VAL A 167	27.289	-10.438	31.381	1.00	46.23	A
ATOM	1310	CA	VAL A 167	26.726	-11.744	31.667	1.00	46.03	A
ATOM	1311	CB	VAL A 167	26.448	-12.542	30.396	1.00	46.87	A
ATOM	1312	CG1	VAL A 167	25.648	-13.784	30.749	1.00	48.77	A
ATOM	1313	CG2	VAL A 167	25.683	-11.675	29.393	1.00	48.21	A
ATOM	1314	C	VAL A 167	27.588	-12.581	32.568	1.00	46.09	A
ATOM	1315	O	VAL A 167	28.672	-13.013	32.191	1.00	48.22	A
ATOM	1316	N	PRO A 168	27.093	-12.836	33.780	1.00	47.27	A
ATOM	1317	CD	PRO A 168	25.763	-12.376	34.217	1.00	46.22	A
ATOM	1318	CA	PRO A 168	27.740	-13.620	34.829	1.00	49.84	A
ATOM	1319	CB	PRO A 168	26.731	-13.552	35.968	1.00	51.34	A
ATOM	1320	CG	PRO A 168	25.408	-13.408	35.241	1.00	48.56	A
ATOM	1321	C	PRO A 168	28.070	-15.055	34.442	1.00	52.74	A
ATOM	1322	O	PRO A 168	27.392	-15.656	33.617	1.00	54.95	A
ATOM	1323	N	PRO A 169	29.122	-15.624	35.048	1.00	56.08	A
ATOM	1324	CD	PRO A 169	30.000	-14.946	36.017	1.00	58.84	A
ATOM	1325	CA	PRO A 169	29.587	-16.993	34.808	1.00	58.16	A
ATOM	1326	CB	PRO A 169	30.693	-17.168	35.849	1.00	58.15	A
ATOM	1327	CG	PRO A 169	31.251	-15.804	35.967	1.00	61.56	A
ATOM	1328	C	PRO A 169	28.466	-17.995	35.025	1.00	58.07	A
ATOM	1329	O	PRO A 169	27.704	-17.871	35.981	1.00	59.45	A
ATOM	1330	N	MET A 170	28.368	-18.987	34.147	1.00	57.55	A
ATOM	1331	CA	MET A 170	27.335	-20.002	34.273	1.00	53.80	A
ATOM	1332	CB	MET A 170	27.779	-21.032	35.303	1.00	53.82	A
ATOM	1333	CG	MET A 170	28.948	-21.857	34.811	1.00	67.88	A
ATOM	1334	SD	MET A 170	29.786	-22.829	36.069	1.00	79.30	A
ATOM	1335	CE	MET A 170	31.340	-21.887	36.209	1.00	77.73	A
ATOM	1336	C	MET A 170	26.009	-19.369	34.673	1.00	52.55	A
ATOM	1337	O	MET A 170	25.255	-19.924	35.477	1.00	50.48	A
ATOM	1338	N	GLY A 171	25.746	-18.194	34.107	1.00	49.32	A
ATOM	1339	CA	GLY A 171	24.524	-17.481	34.394	1.00	51.25	A
ATOM	1340	C	GLY A 171	23.985	-16.844	33.134	1.00	57.47	A
ATOM	1341	O	GLY A 171	24.376	-17.222	32.030	1.00	59.54	A
ATOM	1342	N	GLU A 172	23.095	-15.869	33.289	1.00	60.67	A
ATOM	1343	CA	GLU A 172	22.500	-15.206	32.141	1.00	64.80	A



ATOM	1344	CB	GLU	A	172	21.456	-16.129	31.516	1.00	71.05	A
ATOM	1345	CG	GLU	A	172	20.494	-16.737	32.526	1.00	78.57	A
ATOM	1346	CD	GLU	A	172	19.669	-17.861	31.931	1.00	83.92	A
ATOM	1347	OE1	GLU	A	172	18.875	-17.588	31.004	1.00	84.47	A
ATOM	1348	OE2	GLU	A	172	19.823	-19.019	32.387	1.00	86.75	A
ATOM	1349	C	GLU	A	172	21.870	-13.863	32.481	1.00	64.91	A
ATOM	1350	O	GLU	A	172	21.600	-13.562	33.635	1.00	67.26	A
ATOM	1351	N	SER	A	173	21.632	-13.063	31.453	1.00	66.61	A
ATOM	1352	CA	SER	A	173	21.049	-11.741	31.612	1.00	69.38	A
ATOM	1353	CB	SER	A	173	22.157	-10.690	31.610	1.00	68.94	A
ATOM	1354	OG	SER	A	173	23.337	-11.206	32.208	1.00	74.42	A
ATOM	1355	C	SER	A	173	20.109	-11.482	30.440	1.00	71.97	A
ATOM	1356	O	SER	A	173	20.359	-11.944	29.325	1.00	70.20	A
ATOM	1357	N	ALA	A	174	19.035	-10.742	30.684	1.00	75.48	A
ATOM	1358	CA	ALA	A	174	18.094	-10.442	29.622	1.00	78.56	A
ATOM	1359	CB	ALA	A	174	16.695	-10.921	30.018	1.00	77.27	A
ATOM	1360	C	ALA	A	174	18.063	-8.952	29.289	1.00	81.26	A
ATOM	1361	O	ALA	A	174	17.719	-8.127	30.136	1.00	83.51	A
ATOM	1362	N	VAL	A	175	18.444	-8.611	28.064	1.00	83.71	A
ATOM	1363	CA	VAL	A	175	18.407	-7.230	27.608	1.00	90.85	A
ATOM	1364	CB	VAL	A	175	19.557	-6.926	26.622	1.00	92.75	A
ATOM	1365	CG1	VAL	A	175	19.324	-5.570	25.946	1.00	87.47	A
ATOM	1366	CG2	VAL	A	175	20.900	-6.936	27.336	1.00	93.36	A
ATOM	1367	C	VAL	A	175	17.079	-7.025	26.890	1.00	96.22	A
ATOM	1368	O	VAL	A	175	16.670	-7.869	26.094	1.00	97.56	A
ATOM	1369	N	LYS	A	176	16.406	-5.915	27.188	1.00	99.57	A
ATOM	1370	CA	LYS	A	176	15.111	-5.630	26.573	1.00	103.13	A
ATOM	1371	CB	LYS	A	176	14.599	-4.241	26.970	1.00	101.70	A
ATOM	1372	CG	LYS	A	176	14.200	-4.103	28.450	1.00	104.25	A
ATOM	1373	CD	LYS	A	176	15.409	-4.184	29.395	1.00	100.55	A
ATOM	1374	CE	LYS	A	176	15.046	-3.771	30.825	1.00	93.06	A
ATOM	1375	NZ	LYS	A	176	13.964	-4.622	31.397	1.00	86.44	A
ATOM	1376	C	LYS	A	176	15.210	-5.711	25.048	1.00	107.60	A
ATOM	1377	O	LYS	A	176	15.921	-4.928	24.417	1.00	108.29	A
ATOM	1378	N	LEU	A	177	14.496	-6.673	24.464	1.00	110.94	A
ATOM	1379	CA	LEU	A	177	14.457	-6.886	23.016	1.00	114.23	A
ATOM	1380	CB	LEU	A	177	14.101	-8.349	22.756	1.00	110.63	A
ATOM	1381	CG	LEU	A	177	14.158	-8.910	21.333	1.00	108.29	A
ATOM	1382	CD1	LEU	A	177	15.327	-8.307	20.553	1.00	106.45	A
ATOM	1383	CD2	LEU	A	177	14.307	-10.432	21.404	1.00	106.48	A
ATOM	1384	C	LEU	A	177	13.420	-5.929	22.402	1.00	118.01	A
ATOM	1385	O	LEU	A	177	12.214	-6.091	22.592	1.00	117.68	A
ATOM	1386	N	PRO	A	178	13.894	-4.926	21.642	1.00	121.47	A
ATOM	1387	CD	PRO	A	178	15.313	-4.810	21.255	1.00	122.27	A
ATOM	1388	CA	PRO	A	178	13.107	-3.885	20.971	1.00	124.48	A
ATOM	1389	CB	PRO	A	178	14.183	-2.987	20.376	1.00	122.83	A
ATOM	1390	CG	PRO	A	178	15.233	-3.964	20.001	1.00	124.50	A
ATOM	1391	C	PRO	A	178	12.074	-4.289	19.922	1.00	128.02	A
ATOM	1392	O	PRO	A	178	11.162	-3.513	19.622	1.00	129.47	A
ATOM	1393	N	SER	A	179	12.215	-5.485	19.358	1.00	130.50	A
ATOM	1394	CA	SER	A	179	11.303	-5.984	18.318	1.00	132.08	A
ATOM	1395	CB	SER	A	179	9.832	-5.742	18.705	1.00	132.69	A
ATOM	1396	OG	SER	A	179	8.953	-6.444	17.839	1.00	133.48	A
ATOM	1397	C	SER	A	179	11.598	-5.436	16.910	1.00	132.03	A
ATOM	1398	O	SER	A	179	11.094	-5.964	15.905	1.00	131.83	A
ATOM	1399	N	ASP	A	180	12.398	-4.368	16.846	1.00	131.38	A
ATOM	1400	CA	ASP	A	180	12.847	-3.787	15.568	1.00	129.15	A
ATOM	1401	CB	ASP	A	180	13.446	-2.385	15.784	1.00	129.31	A



ATOM	1402	CG	ASP	A	180	12.441	-1.388	16.322	1.00129.01	A
ATOM	1403	OD1	ASP	A	180	12.834	-0.224	16.593	1.00127.86	A
ATOM	1404	OD2	ASP	A	180	11.256	-1.757	16.465	1.00127.72	A
ATOM	1405	C	ASP	A	180	13.955	-4.772	15.203	1.00127.36	A
ATOM	1406	O	ASP	A	180	14.943	-4.458	14.562	1.00125.75	A
ATOM	1407	N	ALA	A	181	13.708	-5.982	15.682	1.00126.10	A
ATOM	1408	CA	ALA	A	181	14.524	-7.179	15.613	1.00125.36	A
ATOM	1409	CB	ALA	A	181	13.688	-8.331	16.059	1.00123.72	A
ATOM	1410	C	ALA	A	181	15.211	-7.562	14.313	1.00125.78	A
ATOM	1411	O	ALA	A	181	15.593	-6.731	13.486	1.00124.90	A
ATOM	1412	N	GLY	A	182	15.415	-8.874	14.232	1.00126.89	A
ATOM	1413	CA	GLY	A	182	16.050	-9.561	13.124	1.00128.12	A
ATOM	1414	C	GLY	A	182	16.259	-10.982	13.618	1.00128.80	A
ATOM	1415	O	GLY	A	182	15.324	-11.785	13.650	1.00129.69	A
ATOM	1416	N	SER	A	183	17.487	-11.264	14.031	1.00127.74	A
ATOM	1417	CA	SER	A	183	17.896	-12.555	14.548	1.00125.79	A
ATOM	1418	CB	SER	A	183	17.185	-13.710	13.847	1.00126.51	A
ATOM	1419	OG	SER	A	183	17.190	-14.862	14.674	1.00126.57	A
ATOM	1420	C	SER	A	183	19.362	-12.563	14.192	1.00123.68	A
ATOM	1421	O	SER	A	183	20.130	-13.436	14.600	1.00123.14	A
ATOM	1422	N	ASN	A	184	19.731	-11.559	13.405	1.00121.45	A
ATOM	1423	CA	ASN	A	184	21.103	-11.355	12.972	1.00118.98	A
ATOM	1424	CB	ASN	A	184	21.150	-10.362	11.796	1.00119.48	A
ATOM	1425	CG	ASN	A	184	22.571	-10.048	11.346	1.00120.66	A
ATOM	1426	OD1	ASN	A	184	23.311	-10.942	10.927	1.00121.24	A
ATOM	1427	ND2	ASN	A	184	22.959	-8.773	11.435	1.00119.84	A
ATOM	1428	C	ASN	A	184	21.818	-10.771	14.178	1.00115.89	A
ATOM	1429	O	ASN	A	184	22.584	-9.807	14.071	1.00115.71	A
ATOM	1430	N	ILE	A	185	21.531	-11.348	15.338	1.00111.89	A
ATOM	1431	CA	ILE	A	185	22.142	-10.889	16.571	1.00107.91	A
ATOM	1432	CB	ILE	A	185	21.827	-11.843	17.736	1.00106.06	A
ATOM	1433	CG2	ILE	A	185	22.492	-11.332	19.010	1.00107.39	A
ATOM	1434	CG1	ILE	A	185	20.311	-11.935	17.940	1.00100.90	A
ATOM	1435	CD1	ILE	A	185	19.900	-12.804	19.106	1.00 97.34	A
ATOM	1436	C	ILE	A	185	23.656	-10.778	16.393	1.00105.30	A
ATOM	1437	O	ILE	A	185	24.318	-11.727	15.970	1.00105.17	A
ATOM	1438	N	THR	A	186	24.189	-9.603	16.707	1.00100.69	A
ATOM	1439	CA	THR	A	186	25.612	-9.335	16.563	1.00 93.77	A
ATOM	1440	CB	THR	A	186	25.827	-8.411	15.382	1.00 92.19	A
ATOM	1441	OG1	THR	A	186	24.918	-7.307	15.473	1.00 90.68	A
ATOM	1442	CG2	THR	A	186	25.555	-9.146	14.097	1.00 92.78	A
ATOM	1443	C	THR	A	186	26.212	-8.711	17.818	1.00 89.49	A
ATOM	1444	O	THR	A	186	25.590	-7.863	18.462	1.00 88.41	A
ATOM	1445	N	TYR	A	187	27.433	-9.116	18.154	1.00 84.65	A
ATOM	1446	CA	TYR	A	187	28.067	-8.604	19.361	1.00 77.64	A
ATOM	1447	CB	TYR	A	187	27.500	-9.339	20.560	1.00 71.90	A
ATOM	1448	CG	TYR	A	187	27.941	-10.778	20.586	1.00 66.23	A
ATOM	1449	CD1	TYR	A	187	29.201	-11.133	21.061	1.00 65.84	A
ATOM	1450	CE1	TYR	A	187	29.629	-12.451	21.061	1.00 64.03	A
ATOM	1451	CD2	TYR	A	187	27.116	-11.782	20.108	1.00 66.58	A
ATOM	1452	CE2	TYR	A	187	27.535	-13.106	20.101	1.00 67.83	A
ATOM	1453	CZ	TYR	A	187	28.793	-13.432	20.581	1.00 65.88	A
ATOM	1454	OH	TYR	A	187	29.210	-14.741	20.582	1.00 71.57	A
ATOM	1455	C	TYR	A	187	29.572	-8.779	19.395	1.00 74.75	A
ATOM	1456	O	TYR	A	187	30.123	-9.677	18.768	1.00 76.90	A
ATOM	1457	N	ARG	A	188	30.222	-7.920	20.163	1.00 72.05	A
ATOM	1458	CA	ARG	A	188	31.664	-7.984	20.369	1.00 68.17	A
ATOM	1459	CB	ARG	A	188	32.335	-6.736	19.794	1.00 68.30	A



ATOM	1460	CG	ARG	A	188	31.964	-6.447	18.349	1.00	72.52	A
ATOM	1461	CD	ARG	A	188	32.486	-5.094	17.891	1.00	72.57	A
ATOM	1462	NE	ARG	A	188	33.938	-5.063	17.772	1.00	79.20	A
ATOM	1463	CZ	ARG	A	188	34.626	-5.739	16.857	1.00	83.58	A
ATOM	1464	NH1	ARG	A	188	33.991	-6.500	15.978	1.00	84.25	A
ATOM	1465	NH2	ARG	A	188	35.950	-5.654	16.819	1.00	85.58	A
ATOM	1466	C	ARG	A	188	31.759	-7.988	21.898	1.00	64.34	A
ATOM	1467	O	ARG	A	188	30.749	-7.753	22.571	1.00	67.40	A
ATOM	1468	N	THR	A	189	32.921	-8.285	22.468	1.00	55.07	A
ATOM	1469	CA	THR	A	189	33.013	-8.235	23.925	1.00	49.47	A
ATOM	1470	CB	THR	A	189	33.019	-9.605	24.575	1.00	41.74	A
ATOM	1471	OG1	THR	A	189	34.320	-10.186	24.436	1.00	38.57	A
ATOM	1472	CG2	THR	A	189	31.956	-10.483	23.959	1.00	40.69	A
ATOM	1473	C	THR	A	189	34.270	-7.512	24.369	1.00	50.81	A
ATOM	1474	O	THR	A	189	35.010	-6.968	23.545	1.00	53.06	A
ATOM	1475	N	ILE	A	190	34.510	-7.493	25.675	1.00	47.66	A
ATOM	1476	CA	ILE	A	190	35.678	-6.810	26.188	1.00	43.07	A
ATOM	1477	CB	ILE	A	190	35.241	-5.625	27.060	1.00	40.04	A
ATOM	1478	CG2	ILE	A	190	36.442	-4.768	27.443	1.00	37.19	A
ATOM	1479	CG1	ILE	A	190	34.250	-4.776	26.249	1.00	39.66	A
ATOM	1480	CD1	ILE	A	190	33.859	-3.460	26.863	1.00	30.47	A
ATOM	1481	C	ILE	A	190	36.558	-7.796	26.935	1.00	43.76	A
ATOM	1482	O	ILE	A	190	36.153	-8.377	27.942	1.00	46.04	A
ATOM	1483	N	ASN	A	191	37.763	-8.001	26.412	1.00	40.93	A
ATOM	1484	CA	ASN	A	191	38.701	-8.947	27.001	1.00	39.01	A
ATOM	1485	CB	ASN	A	191	39.641	-9.487	25.937	1.00	41.88	A
ATOM	1486	CG	ASN	A	191	40.487	-8.393	25.310	1.00	43.26	A
ATOM	1487	OD1	ASN	A	191	41.093	-7.562	26.002	1.00	42.40	A
ATOM	1488	ND2	ASN	A	191	40.533	-8.389	23.996	1.00	41.76	A
ATOM	1489	C	ASN	A	191	39.550	-8.364	28.110	1.00	36.32	A
ATOM	1490	O	ASN	A	191	39.580	-7.149	28.332	1.00	36.00	A
ATOM	1491	N	ASP	A	192	40.269	-9.269	28.762	1.00	28.92	A
ATOM	1492	CA	ASP	A	192	41.154	-8.971	29.867	1.00	27.52	A
ATOM	1493	CB	ASP	A	192	42.091	-10.152	30.114	1.00	30.28	A
ATOM	1494	CG	ASP	A	192	41.360	-11.413	30.558	1.00	37.35	A
ATOM	1495	OD1	ASP	A	192	42.052	-12.372	30.957	1.00	40.37	A
ATOM	1496	OD2	ASP	A	192	40.112	-11.454	30.512	1.00	40.36	A
ATOM	1497	C	ASP	A	192	42.003	-7.733	29.674	1.00	32.17	A
ATOM	1498	O	ASP	A	192	42.551	-7.200	30.638	1.00	33.76	A
ATOM	1499	N	TYR	A	193	42.127	-7.262	28.441	1.00	34.99	A
ATOM	1500	CA	TYR	A	193	42.965	-6.096	28.196	1.00	36.95	A
ATOM	1501	CB	TYR	A	193	43.944	-6.387	27.060	1.00	38.04	A
ATOM	1502	CG	TYR	A	193	44.606	-7.716	27.256	1.00	38.50	A
ATOM	1503	CD1	TYR	A	193	44.205	-8.827	26.524	1.00	38.64	A
ATOM	1504	CE1	TYR	A	193	44.751	-10.082	26.774	1.00	44.97	A
ATOM	1505	CD2	TYR	A	193	45.576	-7.889	28.246	1.00	43.23	A
ATOM	1506	CE2	TYR	A	193	46.130	-9.134	28.504	1.00	43.94	A
ATOM	1507	CZ	TYR	A	193	45.717	-10.229	27.766	1.00	46.01	A
ATOM	1508	OH	TYR	A	193	46.278	-11.466	28.010	1.00	46.49	A
ATOM	1509	C	TYR	A	193	42.126	-4.900	27.881	1.00	37.64	A
ATOM	1510	O	TYR	A	193	42.625	-3.876	27.408	1.00	38.90	A
ATOM	1511	N	GLY	A	194	40.839	-5.042	28.163	1.00	39.29	A
ATOM	1512	CA	GLY	A	194	39.915	-3.956	27.929	1.00	44.48	A
ATOM	1513	C	GLY	A	194	39.877	-3.675	26.459	1.00	45.55	A
ATOM	1514	O	GLY	A	194	39.659	-2.541	26.039	1.00	39.09	A
ATOM	1515	N	ALA	A	195	40.105	-4.737	25.687	1.00	51.50	A
ATOM	1516	CA	ALA	A	195	40.112	-4.664	24.234	1.00	52.92	A
ATOM	1517	CB	ALA	A	195	41.388	-5.308	23.697	1.00	55.95	A



ATOM	1518	C	ALA	A	195	38.875	-5.363	23.663	1.00	52.17	A
ATOM	1519	O	ALA	A	195	38.416	-6.372	24.204	1.00	44.64	A
ATOM	1520	N	LEU	A	196	38.336	-4.800	22.581	1.00	57.21	A
ATOM	1521	CA	LEU	A	196	37.156	-5.343	21.914	1.00	59.75	A
ATOM	1522	CB	LEU	A	196	36.579	-4.325	20.925	1.00	61.85	A
ATOM	1523	CG	LEU	A	196	35.802	-3.124	21.471	1.00	67.63	A
ATOM	1524	CD1	LEU	A	196	35.470	-2.154	20.342	1.00	69.19	A
ATOM	1525	CD2	LEU	A	196	34.529	-3.609	22.146	1.00	68.00	A
ATOM	1526	C	LEU	A	196	37.511	-6.603	21.152	1.00	60.64	A
ATOM	1527	O	LEU	A	196	38.426	-6.606	20.336	1.00	64.49	A
ATOM	1528	N	THR	A	197	36.797	-7.684	21.417	1.00	62.05	A
ATOM	1529	CA	THR	A	197	37.066	-8.910	20.695	1.00	63.87	A
ATOM	1530	CB	THR	A	197	36.440	-10.133	21.391	1.00	61.93	A
ATOM	1531	OG1	THR	A	197	35.008	-10.042	21.347	1.00	60.47	A
ATOM	1532	CG2	THR	A	197	36.911	-10.204	22.833	1.00	59.69	A
ATOM	1533	C	THR	A	197	36.437	-8.709	19.321	1.00	67.77	A
ATOM	1534	O	THR	A	197	35.717	-7.730	19.097	1.00	64.73	A
ATOM	1535	N	PRO	A	198	36.709	-9.620	18.377	1.00	71.03	A
ATOM	1536	CD	PRO	A	198	37.588	-10.802	18.434	1.00	71.83	A
ATOM	1537	CA	PRO	A	198	36.130	-9.467	17.044	1.00	73.03	A
ATOM	1538	CB	PRO	A	198	36.950	-10.440	16.209	1.00	69.75	A
ATOM	1539	CG	PRO	A	198	37.205	-11.548	17.180	1.00	70.02	A
ATOM	1540	C	PRO	A	198	34.633	-9.778	17.023	1.00	75.14	A
ATOM	1541	O	PRO	A	198	34.160	-10.672	17.733	1.00	76.71	A
ATOM	1542	N	LYS	A	199	33.904	-9.022	16.205	1.00	75.43	A
ATOM	1543	CA	LYS	A	199	32.461	-9.174	16.040	1.00	74.90	A
ATOM	1544	CB	LYS	A	199	31.996	-8.239	14.924	1.00	72.98	A
ATOM	1545	CG	LYS	A	199	30.553	-8.372	14.496	1.00	80.47	A
ATOM	1546	CD	LYS	A	199	30.224	-7.211	13.545	1.00	88.05	A
ATOM	1547	CE	LYS	A	199	29.032	-7.494	12.628	1.00	91.80	A
ATOM	1548	NZ	LYS	A	199	27.748	-7.639	13.354	1.00	91.26	A
ATOM	1549	C	LYS	A	199	32.081	-10.618	15.721	1.00	74.91	A
ATOM	1550	O	LYS	A	199	32.672	-11.243	14.847	1.00	75.65	A
ATOM	1551	N	MET	A	200	31.108	-11.156	16.444	1.00	76.24	A
ATOM	1552	CA	MET	A	200	30.674	-12.524	16.203	1.00	77.12	A
ATOM	1553	CB	MET	A	200	31.023	-13.418	17.390	1.00	79.60	A
ATOM	1554	CG	MET	A	200	32.009	-12.807	18.358	1.00	83.71	A
ATOM	1555	SD	MET	A	200	32.809	-14.062	19.372	1.00	95.64	A
ATOM	1556	CE	MET	A	200	34.534	-13.534	19.211	1.00	90.12	A
ATOM	1557	C	MET	A	200	29.174	-12.514	15.981	1.00	76.38	A
ATOM	1558	O	MET	A	200	28.507	-11.532	16.310	1.00	74.07	A
ATOM	1559	N	THR	A	201	28.647	-13.606	15.430	1.00	77.03	A
ATOM	1560	CA	THR	A	201	27.219	-13.702	15.148	1.00	78.59	A
ATOM	1561	CB	THR	A	201	26.962	-14.410	13.799	1.00	77.42	A
ATOM	1562	OG1	THR	A	201	27.594	-13.670	12.749	1.00	77.17	A
ATOM	1563	CG2	THR	A	201	25.465	-14.496	13.516	1.00	74.13	A
ATOM	1564	C	THR	A	201	26.408	-14.412	16.221	1.00	79.06	A
ATOM	1565	O	THR	A	201	26.785	-15.482	16.703	1.00	78.93	A
ATOM	1566	N	GLY	A	202	25.282	-13.803	16.575	1.00	80.08	A
ATOM	1567	CA	GLY	A	202	24.406	-14.374	17.576	1.00	85.07	A
ATOM	1568	C	GLY	A	202	23.994	-15.781	17.203	1.00	88.30	A
ATOM	1569	O	GLY	A	202	23.627	-16.041	16.056	1.00	89.73	A
ATOM	1570	N	VAL	A	203	24.048	-16.684	18.177	1.00	89.55	A
ATOM	1571	CA	VAL	A	203	23.701	-18.083	17.958	1.00	91.19	A
ATOM	1572	CB	VAL	A	203	24.965	-18.955	18.037	1.00	90.44	A
ATOM	1573	CG1	VAL	A	203	24.639	-20.396	17.682	1.00	89.78	A
ATOM	1574	CG2	VAL	A	203	26.028	-18.389	17.119	1.00	88.29	A
ATOM	1575	C	VAL	A	203	22.691	-18.579	18.993	1.00	93.60	A



ATOM	1576	O	VAL	A	203	23.051	-19.320	19.910	1.00	96.46	A
ATOM	1577	N	MET	A	204	21.432	-18.173	18.837	1.00	94.45	A
ATOM	1578	CA	MET	A	204	20.359	-18.554	19.763	1.00	95.79	A
ATOM	1579	CB	MET	A	204	18.988	-18.259	19.139	1.00	97.75	A
ATOM	1580	CG	MET	A	204	18.717	-16.781	18.846	1.00	100.91	A
ATOM	1581	SD	MET	A	204	19.848	-16.028	17.632	1.00	110.31	A
ATOM	1582	CE	MET	A	204	19.018	-16.409	16.081	1.00	106.42	A
ATOM	1583	C	MET	A	204	20.419	-20.022	20.175	1.00	95.44	A
ATOM	1584	O	MET	A	204	20.568	-20.902	19.337	1.00	94.73	A
ATOM	1585	N	GLU	A	205	20.304	-20.282	21.471	1.00	97.70	A
ATOM	1586	CA	GLU	A	205	20.343	-21.651	21.968	1.00	101.28	A
ATOM	1587	CB	GLU	A	205	20.877	-21.711	23.403	1.00	104.84	A
ATOM	1588	CG	GLU	A	205	19.906	-21.187	24.466	1.00	112.54	A
ATOM	1589	CD	GLU	A	205	19.661	-22.185	25.597	1.00	116.36	A
ATOM	1590	OE1	GLU	A	205	18.893	-21.859	26.535	1.00	117.19	A
ATOM	1591	OE2	GLU	A	205	20.234	-23.296	25.544	1.00	117.69	A
ATOM	1592	C	GLU	A	205	18.933	-22.211	21.939	1.00	102.68	A
ATOM	1593	O	GLU	A	205	18.782	-23.396	21.575	1.00	102.57	A
ATOM	1594	OXT	GLU	A	205	18.003	-21.453	22.299	1.00	103.89	A
ATOM	1595	CB	PHE	B	1	82.345	-11.695	6.773	1.00	32.64	B
ATOM	1596	CG	PHE	B	1	81.373	-11.042	7.714	1.00	34.25	B
ATOM	1597	CD1	PHE	B	1	80.035	-10.867	7.347	1.00	36.18	B
ATOM	1598	CD2	PHE	B	1	81.769	-10.662	8.993	1.00	31.51	B
ATOM	1599	CE1	PHE	B	1	79.108	-10.333	8.242	1.00	29.96	B
ATOM	1600	CE2	PHE	B	1	80.847	-10.122	9.898	1.00	30.37	B
ATOM	1601	CZ	PHE	B	1	79.514	-9.962	9.519	1.00	32.63	B
ATOM	1602	C	PHE	B	1	80.968	-13.803	6.514	1.00	32.70	B
ATOM	1603	O	PHE	B	1	80.485	-13.669	5.389	1.00	29.68	B
ATOM	1604	N	PHE	B	1	83.310	-13.795	5.858	1.00	39.65	B
ATOM	1605	CA	PHE	B	1	82.342	-13.237	6.842	1.00	35.44	B
ATOM	1606	N	ALA	B	2	80.360	-14.460	7.496	1.00	31.71	B
ATOM	1607	CA	ALA	B	2	79.040	-15.055	7.321	1.00	30.82	B
ATOM	1608	CB	ALA	B	2	79.189	-16.485	6.894	1.00	21.90	B
ATOM	1609	C	ALA	B	2	78.259	-14.976	8.631	1.00	30.47	B
ATOM	1610	O	ALA	B	2	78.859	-14.856	9.707	1.00	29.13	B
ATOM	1611	N	CYS	B	3	76.932	-15.045	8.549	1.00	24.69	B
ATOM	1612	CA	CYS	B	3	76.126	-14.973	9.755	1.00	25.87	B
ATOM	1613	C	CYS	B	3	75.086	-16.076	9.766	1.00	25.80	B
ATOM	1614	O	CYS	B	3	74.775	-16.636	8.731	1.00	27.41	B
ATOM	1615	CB	CYS	B	3	75.430	-13.618	9.847	1.00	29.97	B
ATOM	1616	SG	CYS	B	3	76.471	-12.127	9.708	1.00	38.20	B
ATOM	1617	N	LYS	B	4	74.554	-16.390	10.942	1.00	28.12	B
ATOM	1618	CA	LYS	B	4	73.531	-17.423	11.060	1.00	31.79	B
ATOM	1619	CB	LYS	B	4	74.120	-18.786	11.447	1.00	28.60	B
ATOM	1620	CG	LYS	B	4	74.710	-18.828	12.846	1.00	40.21	B
ATOM	1621	CD	LYS	B	4	75.426	-20.146	13.165	1.00	46.80	B
ATOM	1622	CE	LYS	B	4	74.462	-21.313	13.324	1.00	57.63	B
ATOM	1623	NZ	LYS	B	4	73.773	-21.671	12.052	1.00	66.21	B
ATOM	1624	C	LYS	B	4	72.502	-17.025	12.096	1.00	34.54	B
ATOM	1625	O	LYS	B	4	72.742	-16.198	12.972	1.00	33.51	B
ATOM	1626	N	THR	B	5	71.348	-17.653	11.982	1.00	36.23	B
ATOM	1627	CA	THR	B	5	70.242	-17.395	12.852	1.00	35.55	B
ATOM	1628	CB	THR	B	5	68.965	-17.255	11.990	1.00	33.20	B
ATOM	1629	OG1	THR	B	5	68.279	-16.064	12.371	1.00	39.62	B
ATOM	1630	CG2	THR	B	5	68.068	-18.440	12.114	1.00	21.80	B
ATOM	1631	C	THR	B	5	70.167	-18.515	13.873	1.00	36.29	B
ATOM	1632	O	THR	B	5	70.353	-19.685	13.544	1.00	39.71	B
ATOM	1633	N	ALA	B	6	69.941	-18.141	15.124	1.00	37.36	B



ATOM	1634	CA	ALA	B	6	69.854	-19.100	16.217	1.00	37.84	B
ATOM	1635	CB	ALA	B	6	69.476	-18.389	17.505	1.00	37.58	B
ATOM	1636	C	ALA	B	6	68.840	-20.172	15.907	1.00	41.46	B
ATOM	1637	O	ALA	B	6	68.921	-21.289	16.413	1.00	43.45	B
ATOM	1638	N	ASN	B	7	67.877	-19.830	15.064	1.00	48.11	B
ATOM	1639	CA	ASN	B	7	66.832	-20.774	14.690	1.00	52.20	B
ATOM	1640	CB	ASN	B	7	65.690	-20.040	14.008	1.00	54.22	B
ATOM	1641	CG	ASN	B	7	64.345	-20.578	14.405	1.00	55.97	B
ATOM	1642	OD1	ASN	B	7	64.253	-21.579	15.121	1.00	57.99	B
ATOM	1643	ND2	ASN	B	7	63.286	-19.920	13.945	1.00	50.39	B
ATOM	1644	C	ASN	B	7	67.372	-21.833	13.756	1.00	51.16	B
ATOM	1645	O	ASN	B	7	66.973	-22.998	13.824	1.00	55.83	B
ATOM	1646	N	GLY	B	8	68.277	-21.410	12.884	1.00	50.20	B
ATOM	1647	CA	GLY	B	8	68.889	-22.318	11.940	1.00	55.38	B
ATOM	1648	C	GLY	B	8	69.492	-21.649	10.708	1.00	59.62	B
ATOM	1649	O	GLY	B	8	70.656	-21.908	10.370	1.00	62.92	B
ATOM	1650	N	THR	B	9	68.716	-20.777	10.055	1.00	54.57	B
ATOM	1651	CA	THR	B	9	69.120	-20.093	8.820	1.00	49.33	B
ATOM	1652	CB	THR	B	9	67.975	-19.233	8.317	1.00	48.69	B
ATOM	1653	OG1	THR	B	9	66.818	-20.062	8.173	1.00	56.73	B
ATOM	1654	CG2	THR	B	9	68.309	-18.617	6.976	1.00	49.41	B
ATOM	1655	C	THR	B	9	70.405	-19.265	8.772	1.00	47.43	B
ATOM	1656	O	THR	B	9	70.772	-18.598	9.733	1.00	49.84	B
ATOM	1657	N	ALA	B	10	71.071	-19.311	7.617	1.00	43.83	B
ATOM	1658	CA	ALA	B	10	72.330	-18.606	7.394	1.00	39.16	B
ATOM	1659	CB	ALA	B	10	73.463	-19.607	7.265	1.00	31.66	B
ATOM	1660	C	ALA	B	10	72.323	-17.741	6.159	1.00	37.14	B
ATOM	1661	O	ALA	B	10	71.521	-17.942	5.252	1.00	38.98	B
ATOM	1662	N	ILE	B	11	73.223	-16.767	6.144	1.00	32.97	B
ATOM	1663	CA	ILE	B	11	73.404	-15.896	5.001	1.00	33.22	B
ATOM	1664	CB	ILE	B	11	73.107	-14.448	5.317	1.00	34.97	B
ATOM	1665	CG2	ILE	B	11	73.322	-13.616	4.063	1.00	33.99	B
ATOM	1666	CG1	ILE	B	11	71.671	-14.320	5.838	1.00	36.23	B
ATOM	1667	CD1	ILE	B	11	71.260	-12.903	6.198	1.00	35.08	B
ATOM	1668	C	ILE	B	11	74.881	-16.060	4.767	1.00	33.83	B
ATOM	1669	O	ILE	B	11	75.690	-15.729	5.617	1.00	43.80	B
ATOM	1670	N	PRO	B	12	75.260	-16.575	3.609	1.00	30.79	B
ATOM	1671	CD	PRO	B	12	74.399	-16.999	2.492	1.00	34.49	B
ATOM	1672	CA	PRO	B	12	76.667	-16.797	3.290	1.00	31.29	B
ATOM	1673	CB	PRO	B	12	76.582	-17.816	2.164	1.00	33.05	B
ATOM	1674	CG	PRO	B	12	75.408	-17.288	1.380	1.00	29.85	B
ATOM	1675	C	PRO	B	12	77.503	-15.596	2.889	1.00	32.87	B
ATOM	1676	O	PRO	B	12	77.002	-14.472	2.791	1.00	32.44	B
ATOM	1677	N	ILE	B	13	78.790	-15.881	2.657	1.00	32.91	B
ATOM	1678	CA	ILE	B	13	79.795	-14.910	2.205	1.00	32.69	B
ATOM	1679	CB	ILE	B	13	81.097	-15.633	1.778	1.00	32.47	B
ATOM	1680	CG2	ILE	B	13	82.005	-14.688	0.989	1.00	30.76	B
ATOM	1681	CG1	ILE	B	13	81.800	-16.194	3.018	1.00	30.76	B
ATOM	1682	CD1	ILE	B	13	83.024	-16.954	2.715	1.00	22.14	B
ATOM	1683	C	ILE	B	13	79.229	-14.195	0.989	1.00	31.24	B
ATOM	1684	O	ILE	B	13	78.743	-14.851	0.082	1.00	35.40	B
ATOM	1685	N	GLY	B	14	79.284	-12.868	0.970	1.00	27.66	B
ATOM	1686	CA	GLY	B	14	78.745	-12.129	-0.159	1.00	29.28	B
ATOM	1687	C	GLY	B	14	77.392	-11.498	0.150	1.00	33.58	B
ATOM	1688	O	GLY	B	14	76.859	-10.704	-0.631	1.00	32.37	B
ATOM	1689	N	GLY	B	15	76.817	-11.867	1.289	1.00	34.26	B
ATOM	1690	CA	GLY	B	15	75.543	-11.294	1.676	1.00	32.52	B
ATOM	1691	C	GLY	B	15	74.313	-12.041	1.202	1.00	33.57	B



ATOM	1692	O	GLY	B	15	74.405	-13.053	0.513	1.00	35.21	B
ATOM	1693	N	GLY	B	16	73.150	-11.514	1.577	1.00	30.98	B
ATOM	1694	CA	GLY	B	16	71.887	-12.126	1.224	1.00	23.66	B
ATOM	1695	C	GLY	B	16	70.874	-11.761	2.281	1.00	22.40	B
ATOM	1696	O	GLY	B	16	71.011	-10.742	2.944	1.00	26.18	B
ATOM	1697	N	SER	B	17	69.866	-12.584	2.492	1.00	19.46	B
ATOM	1698	CA	SER	B	17	68.879	-12.199	3.478	1.00	19.03	B
ATOM	1699	CB	SER	B	17	67.775	-11.375	2.796	1.00	25.66	B
ATOM	1700	OG	SER	B	17	66.918	-12.199	2.016	1.00	32.12	B
ATOM	1701	C	SER	B	17	68.265	-13.369	4.197	1.00	16.25	B
ATOM	1702	O	SER	B	17	68.250	-14.476	3.679	1.00	18.07	B
ATOM	1703	N	ALA	B	18	67.746	-13.124	5.396	1.00	15.13	B
ATOM	1704	CA	ALA	B	18	67.115	-14.188	6.160	1.00	13.99	B
ATOM	1705	CB	ALA	B	18	68.153	-14.934	6.969	1.00	11.08	B
ATOM	1706	C	ALA	B	18	66.043	-13.676	7.073	1.00	19.72	B
ATOM	1707	O	ALA	B	18	66.026	-12.498	7.438	1.00	26.53	B
ATOM	1708	N	ASN	B	19	65.145	-14.582	7.439	1.00	20.77	B
ATOM	1709	CA	ASN	B	19	64.054	-14.275	8.344	1.00	19.46	B
ATOM	1710	CB	ASN	B	19	62.847	-15.181	8.073	1.00	15.18	B
ATOM	1711	CG	ASN	B	19	62.037	-14.739	6.870	1.00	18.55	B
ATOM	1712	OD1	ASN	B	19	62.378	-13.761	6.202	1.00	11.36	B
ATOM	1713	ND2	ASN	B	19	60.955	-15.464	6.584	1.00	8.90	B
ATOM	1714	C	ASN	B	19	64.495	-14.532	9.764	1.00	22.89	B
ATOM	1715	O	ASN	B	19	65.205	-15.491	10.038	1.00	25.04	B
ATOM	1716	N	VAL	B	20	64.067	-13.682	10.681	1.00	26.63	B
ATOM	1717	CA	VAL	B	20	64.379	-13.907	12.078	1.00	28.04	B
ATOM	1718	CB	VAL	B	20	65.314	-12.842	12.589	1.00	27.80	B
ATOM	1719	CG1	VAL	B	20	65.751	-13.190	14.000	1.00	29.15	B
ATOM	1720	CG2	VAL	B	20	66.503	-12.759	11.663	1.00	18.43	B
ATOM	1721	C	VAL	B	20	63.054	-13.885	12.840	1.00	26.89	B
ATOM	1722	O	VAL	B	20	62.409	-12.845	12.935	1.00	30.11	B
ATOM	1723	N	TYR	B	21	62.647	-15.041	13.355	1.00	24.58	B
ATOM	1724	CA	TYR	B	21	61.377	-15.181	14.091	1.00	27.54	B
ATOM	1725	CB	TYR	B	21	60.782	-16.553	13.802	1.00	17.79	B
ATOM	1726	CG	TYR	B	21	60.728	-16.848	12.333	1.00	25.42	B
ATOM	1727	CD1	TYR	B	21	61.670	-17.673	11.741	1.00	20.36	B
ATOM	1728	CE1	TYR	B	21	61.642	-17.918	10.364	1.00	28.24	B
ATOM	1729	CD2	TYR	B	21	59.746	-16.266	11.513	1.00	28.10	B
ATOM	1730	CE2	TYR	B	21	59.707	-16.505	10.141	1.00	26.58	B
ATOM	1731	CZ	TYR	B	21	60.659	-17.335	9.575	1.00	31.58	B
ATOM	1732	OH	TYR	B	21	60.605	-17.607	8.234	1.00	35.73	B
ATOM	1733	C	TYR	B	21	61.478	-14.973	15.615	1.00	30.70	B
ATOM	1734	O	TYR	B	21	62.146	-15.747	16.321	1.00	33.69	B
ATOM	1735	N	VAL	B	22	60.783	-13.952	16.122	1.00	29.81	B
ATOM	1736	CA	VAL	B	22	60.842	-13.611	17.550	1.00	28.88	B
ATOM	1737	CB	VAL	B	22	61.344	-12.189	17.758	1.00	26.70	B
ATOM	1738	CG1	VAL	B	22	62.714	-12.019	17.142	1.00	27.48	B
ATOM	1739	CG2	VAL	B	22	60.351	-11.227	17.160	1.00	18.87	B
ATOM	1740	C	VAL	B	22	59.568	-13.677	18.362	1.00	29.53	B
ATOM	1741	O	VAL	B	22	58.531	-13.181	17.931	1.00	29.65	B
ATOM	1742	N	ASN	B	23	59.663	-14.266	19.554	1.00	31.41	B
ATOM	1743	CA	ASN	B	23	58.530	-14.333	20.478	1.00	32.32	B
ATOM	1744	CB	ASN	B	23	58.638	-15.560	21.343	1.00	33.67	B
ATOM	1745	CG	ASN	B	23	59.048	-16.761	20.566	1.00	34.47	B
ATOM	1746	OD1	ASN	B	23	58.219	-17.500	20.030	1.00	31.16	B
ATOM	1747	ND2	ASN	B	23	60.349	-16.960	20.474	1.00	42.29	B
ATOM	1748	C	ASN	B	23	58.675	-13.088	21.353	1.00	32.53	B
ATOM	1749	O	ASN	B	23	59.720	-12.881	21.971	1.00	27.61	B



ATOM	1750	N	LEU	B	24	57.639	-12.258	21.392	1.00	33.86	B
ATOM	1751	CA	LEU	B	24	57.683	-11.015	22.166	1.00	34.98	B
ATOM	1752	CB	LEU	B	24	57.233	-9.857	21.273	1.00	33.61	B
ATOM	1753	CG	LEU	B	24	57.914	-9.705	19.909	1.00	25.28	B
ATOM	1754	CD1	LEU	B	24	56.962	-9.013	18.959	1.00	19.99	B
ATOM	1755	CD2	LEU	B	24	59.196	-8.912	20.028	1.00	29.84	B
ATOM	1756	C	LEU	B	24	56.796	-11.047	23.416	1.00	34.24	B
ATOM	1757	O	LEU	B	24	55.865	-11.849	23.500	1.00	38.70	B
ATOM	1758	N	ALA	B	25	57.086	-10.181	24.386	1.00	29.44	B
ATOM	1759	CA	ALA	B	25	56.266	-10.087	25.601	1.00	26.87	B
ATOM	1760	CB	ALA	B	25	56.657	-8.867	26.375	1.00	21.78	B
ATOM	1761	C	ALA	B	25	54.814	-9.958	25.138	1.00	29.09	B
ATOM	1762	O	ALA	B	25	54.484	-9.078	24.361	1.00	36.37	B
ATOM	1763	N	PRO	B	26	53.924	-10.814	25.619	1.00	27.06	B
ATOM	1764	CD	PRO	B	26	54.129	-11.844	26.637	1.00	28.83	B
ATOM	1765	CA	PRO	B	26	52.513	-10.761	25.206	1.00	31.81	B
ATOM	1766	CB	PRO	B	26	51.888	-11.976	25.921	1.00	32.26	B
ATOM	1767	CG	PRO	B	26	53.043	-12.835	26.271	1.00	36.18	B
ATOM	1768	C	PRO	B	26	51.726	-9.473	25.512	1.00	32.59	B
ATOM	1769	O	PRO	B	26	50.748	-9.150	24.825	1.00	27.68	B
ATOM	1770	N	VAL	B	27	52.154	-8.766	26.553	1.00	33.23	B
ATOM	1771	CA	VAL	B	27	51.508	-7.548	27.009	1.00	30.33	B
ATOM	1772	CB	VAL	B	27	50.729	-7.814	28.299	1.00	32.83	B
ATOM	1773	CG1	VAL	B	27	50.191	-6.519	28.863	1.00	34.49	B
ATOM	1774	CG2	VAL	B	27	49.615	-8.812	28.038	1.00	34.69	B
ATOM	1775	C	VAL	B	27	52.517	-6.468	27.327	1.00	31.47	B
ATOM	1776	O	VAL	B	27	53.525	-6.720	27.968	1.00	36.58	B
ATOM	1777	N	VAL	B	28	52.228	-5.250	26.907	1.00	33.06	B
ATOM	1778	CA	VAL	B	28	53.110	-4.131	27.175	1.00	34.52	B
ATOM	1779	CB	VAL	B	28	54.048	-3.875	25.979	1.00	33.98	B
ATOM	1780	CG1	VAL	B	28	55.047	-2.765	26.297	1.00	34.51	B
ATOM	1781	CG2	VAL	B	28	54.775	-5.146	25.634	1.00	35.52	B
ATOM	1782	C	VAL	B	28	52.183	-2.944	27.391	1.00	39.51	B
ATOM	1783	O	VAL	B	28	51.196	-2.778	26.663	1.00	42.77	B
ATOM	1784	N	ASN	B	29	52.488	-2.123	28.392	1.00	39.90	B
ATOM	1785	CA	ASN	B	29	51.639	-0.977	28.695	1.00	38.73	B
ATOM	1786	CB	ASN	B	29	51.529	-0.748	30.199	1.00	31.74	B
ATOM	1787	CG	ASN	B	29	51.026	-1.952	30.926	1.00	35.82	B
ATOM	1788	OD1	ASN	B	29	49.958	-2.465	30.611	1.00	38.41	B
ATOM	1789	ND2	ASN	B	29	51.794	-2.425	31.910	1.00	41.70	B
ATOM	1790	C	ASN	B	29	52.186	0.275	28.088	1.00	38.86	B
ATOM	1791	O	ASN	B	29	53.385	0.374	27.815	1.00	33.54	B
ATOM	1792	N	VAL	B	30	51.292	1.237	27.891	1.00	37.78	B
ATOM	1793	CA	VAL	B	30	51.695	2.513	27.354	1.00	38.82	B
ATOM	1794	CB	VAL	B	30	50.525	3.522	27.378	1.00	37.94	B
ATOM	1795	CG1	VAL	B	30	50.989	4.887	26.880	1.00	30.95	B
ATOM	1796	CG2	VAL	B	30	49.387	3.013	26.507	1.00	35.51	B
ATOM	1797	C	VAL	B	30	52.773	2.949	28.334	1.00	41.89	B
ATOM	1798	O	VAL	B	30	52.678	2.651	29.526	1.00	37.14	B
ATOM	1799	N	GLY	B	31	53.813	3.610	27.832	1.00	45.72	B
ATOM	1800	CA	GLY	B	31	54.879	4.066	28.706	1.00	48.04	B
ATOM	1801	C	GLY	B	31	56.019	3.080	28.893	1.00	50.10	B
ATOM	1802	O	GLY	B	31	57.159	3.493	29.086	1.00	52.11	B
ATOM	1803	N	GLN	B	32	55.726	1.785	28.841	1.00	49.45	B
ATOM	1804	CA	GLN	B	32	56.755	0.765	29.009	1.00	50.86	B
ATOM	1805	CB	GLN	B	32	56.115	-0.528	29.500	1.00	51.28	B
ATOM	1806	CG	GLN	B	32	56.016	-0.625	31.006	1.00	63.66	B
ATOM	1807	CD	GLN	B	32	55.049	-1.711	31.456	1.00	69.42	B



ATOM	1808	OE1	GLN	B	32	55.004	-2.806	30.875	1.00	67.50	B
ATOM	1809	NE2	GLN	B	32	54.271	-1.417	32.506	1.00	69.01	B
ATOM	1810	C	GLN	B	32	57.578	0.477	27.744	1.00	52.35	B
ATOM	1811	O	GLN	B	32	57.339	1.044	26.673	1.00	52.23	B
ATOM	1812	N	ASN	B	33	58.560	-0.408	27.892	1.00	49.97	B
ATOM	1813	CA	ASN	B	33	59.431	-0.804	26.791	1.00	45.57	B
ATOM	1814	CB	ASN	B	33	60.894	-0.644	27.186	1.00	38.58	B
ATOM	1815	CG	ASN	B	33	61.487	0.663	26.722	1.00	42.92	B
ATOM	1816	OD1	ASN	B	33	62.591	1.031	27.126	1.00	40.10	B
ATOM	1817	ND2	ASN	B	33	60.774	1.367	25.854	1.00	40.86	B
ATOM	1818	C	ASN	B	33	59.230	-2.245	26.341	1.00	46.44	B
ATOM	1819	O	ASN	B	33	59.157	-3.180	27.144	1.00	46.81	B
ATOM	1820	N	LEU	B	34	59.105	-2.418	25.039	1.00	49.23	B
ATOM	1821	CA	LEU	B	34	59.007	-3.747	24.470	1.00	48.60	B
ATOM	1822	CB	LEU	B	34	58.045	-3.774	23.293	1.00	48.20	B
ATOM	1823	CG	LEU	B	34	58.103	-5.057	22.473	1.00	45.79	B
ATOM	1824	CD1	LEU	B	34	57.402	-6.200	23.193	1.00	41.87	B
ATOM	1825	CD2	LEU	B	34	57.451	-4.778	21.133	1.00	49.38	B
ATOM	1826	C	LEU	B	34	60.445	-3.902	23.976	1.00	48.23	B
ATOM	1827	O	LEU	B	34	60.992	-3.012	23.298	1.00	41.48	B
ATOM	1828	N	VAL	B	35	61.077	-5.005	24.334	1.00	47.30	B
ATOM	1829	CA	VAL	B	35	62.450	-5.185	23.916	1.00	47.76	B
ATOM	1830	CB	VAL	B	35	63.375	-5.332	25.139	1.00	51.29	B
ATOM	1831	CG1	VAL	B	35	64.819	-5.444	24.689	1.00	50.08	B
ATOM	1832	CG2	VAL	B	35	63.200	-4.128	26.056	1.00	46.83	B
ATOM	1833	C	VAL	B	35	62.644	-6.368	22.998	1.00	42.61	B
ATOM	1834	O	VAL	B	35	62.279	-7.497	23.333	1.00	42.72	B
ATOM	1835	N	VAL	B	36	63.201	-6.098	21.824	1.00	38.28	B
ATOM	1836	CA	VAL	B	36	63.474	-7.164	20.867	1.00	37.43	B
ATOM	1837	CB	VAL	B	36	62.937	-6.861	19.477	1.00	35.42	B
ATOM	1838	CG1	VAL	B	36	62.693	-8.158	18.759	1.00	38.88	B
ATOM	1839	CG2	VAL	B	36	61.674	-6.048	19.570	1.00	32.55	B
ATOM	1840	C	VAL	B	36	64.974	-7.229	20.790	1.00	36.36	B
ATOM	1841	O	VAL	B	36	65.614	-6.363	20.186	1.00	36.91	B
ATOM	1842	N	ASP	B	37	65.544	-8.241	21.429	1.00	37.46	B
ATOM	1843	CA	ASP	B	37	66.993	-8.380	21.442	1.00	40.31	B
ATOM	1844	CB	ASP	B	37	67.456	-8.800	22.835	1.00	44.25	B
ATOM	1845	CG	ASP	B	37	68.953	-8.744	22.984	1.00	52.42	B
ATOM	1846	OD1	ASP	B	37	69.557	-7.715	22.582	1.00	55.50	B
ATOM	1847	OD2	ASP	B	37	69.523	-9.726	23.506	1.00	58.75	B
ATOM	1848	C	ASP	B	37	67.473	-9.382	20.404	1.00	35.79	B
ATOM	1849	O	ASP	B	37	67.346	-10.593	20.587	1.00	35.22	B
ATOM	1850	N	LEU	B	38	68.039	-8.875	19.318	1.00	33.36	B
ATOM	1851	CA	LEU	B	38	68.506	-9.757	18.255	1.00	38.32	B
ATOM	1852	CB	LEU	B	38	68.451	-9.022	16.917	1.00	34.94	B
ATOM	1853	CG	LEU	B	38	66.983	-8.711	16.654	1.00	28.92	B
ATOM	1854	CD1	LEU	B	38	66.877	-7.753	15.538	1.00	45.30	B
ATOM	1855	CD2	LEU	B	38	66.230	-9.975	16.340	1.00	28.07	B
ATOM	1856	C	LEU	B	38	69.875	-10.374	18.487	1.00	36.75	B
ATOM	1857	O	LEU	B	38	70.201	-11.406	17.886	1.00	32.86	B
ATOM	1858	N	SER	B	39	70.645	-9.748	19.378	1.00	38.02	B
ATOM	1859	CA	SER	B	39	71.982	-10.218	19.760	1.00	36.96	B
ATOM	1860	CB	SER	B	39	72.558	-9.367	20.880	1.00	42.14	B
ATOM	1861	OG	SER	B	39	72.044	-9.821	22.122	1.00	40.54	B
ATOM	1862	C	SER	B	39	71.822	-11.615	20.305	1.00	30.79	B
ATOM	1863	O	SER	B	39	72.785	-12.321	20.531	1.00	33.51	B
ATOM	1864	N	THR	B	40	70.587	-12.000	20.545	1.00	29.18	B
ATOM	1865	CA	THR	B	40	70.327	-13.322	21.042	1.00	28.75	B



ATOM	1866	CB	THR	B	40	69.186	-13.277	22.071	1.00	29.43	B
ATOM	1867	OG1	THR	B	40	69.692	-13.707	23.334	1.00	32.38	B
ATOM	1868	CG2	THR	B	40	68.022	-14.163	21.664	1.00	22.59	B
ATOM	1869	C	THR	B	40	69.961	-14.233	19.890	1.00	29.83	B
ATOM	1870	O	THR	B	40	69.914	-15.457	20.046	1.00	29.41	B
ATOM	1871	N	GLN	B	41	69.718	-13.646	18.721	1.00	31.06	B
ATOM	1872	CA	GLN	B	41	69.313	-14.460	17.582	1.00	36.78	B
ATOM	1873	CB	GLN	B	41	67.847	-14.194	17.264	1.00	40.36	B
ATOM	1874	CG	GLN	B	41	66.926	-14.642	18.369	1.00	43.67	B
ATOM	1875	CD	GLN	B	41	65.703	-15.289	17.820	1.00	52.52	B
ATOM	1876	OE1	GLN	B	41	64.783	-14.617	17.328	1.00	56.24	B
ATOM	1877	NE2	GLN	B	41	65.681	-16.615	17.863	1.00	60.45	B
ATOM	1878	C	GLN	B	41	70.123	-14.351	16.301	1.00	36.15	B
ATOM	1879	O	GLN	B	41	69.910	-15.132	15.372	1.00	31.94	B
ATOM	1880	N	ILE	B	42	71.052	-13.402	16.250	1.00	33.39	B
ATOM	1881	CA	ILE	B	42	71.861	-13.220	15.052	1.00	32.83	B
ATOM	1882	CB	ILE	B	42	71.470	-11.927	14.339	1.00	29.07	B
ATOM	1883	CG2	ILE	B	42	72.264	-11.772	13.064	1.00	37.11	B
ATOM	1884	CG1	ILE	B	42	69.985	-11.956	14.008	1.00	29.91	B
ATOM	1885	CD1	ILE	B	42	69.482	-10.650	13.455	1.00	32.72	B
ATOM	1886	C	ILE	B	42	73.357	-13.207	15.363	1.00	35.46	B
ATOM	1887	O	ILE	B	42	73.854	-12.349	16.108	1.00	34.54	B
ATOM	1888	N	PHE	B	43	74.066	-14.168	14.773	1.00	39.21	B
ATOM	1889	CA	PHE	B	43	75.508	-14.328	14.971	1.00	38.93	B
ATOM	1890	CB	PHE	B	43	75.788	-15.645	15.676	1.00	35.81	B
ATOM	1891	CG	PHE	B	43	75.097	-15.776	16.979	1.00	37.08	B
ATOM	1892	CD1	PHE	B	43	73.774	-16.211	17.038	1.00	36.05	B
ATOM	1893	CD2	PHE	B	43	75.744	-15.399	18.158	1.00	39.14	B
ATOM	1894	CE1	PHE	B	43	73.096	-16.266	18.256	1.00	37.91	B
ATOM	1895	CE2	PHE	B	43	75.084	-15.448	19.382	1.00	40.87	B
ATOM	1896	CZ	PHE	B	43	73.752	-15.882	19.435	1.00	40.29	B
ATOM	1897	C	PHE	B	43	76.342	-14.288	13.706	1.00	38.93	B
ATOM	1898	O	PHE	B	43	75.952	-14.807	12.667	1.00	42.09	B
ATOM	1899	N	CYS	B	44	77.510	-13.681	13.806	1.00	39.28	B
ATOM	1900	CA	CYS	B	44	78.413	-13.609	12.672	1.00	41.35	B
ATOM	1901	C	CYS	B	44	79.836	-14.004	13.111	1.00	42.43	B
ATOM	1902	O	CYS	B	44	80.124	-14.157	14.304	1.00	41.46	B
ATOM	1903	CB	CYS	B	44	78.417	-12.201	12.097	1.00	42.60	B
ATOM	1904	SG	CYS	B	44	76.786	-11.538	11.633	1.00	48.45	B
ATOM	1905	N	HIS	B	45	80.719	-14.192	12.141	1.00	41.61	B
ATOM	1906	CA	HIS	B	45	82.091	-14.563	12.440	1.00	38.21	B
ATOM	1907	CB	HIS	B	45	82.222	-16.073	12.632	1.00	35.18	B
ATOM	1908	CG	HIS	B	45	82.034	-16.856	11.372	1.00	40.84	B
ATOM	1909	CD2	HIS	B	45	82.782	-16.926	10.244	1.00	42.07	B
ATOM	1910	ND1	HIS	B	45	80.931	-17.648	11.146	1.00	43.80	B
ATOM	1911	CE1	HIS	B	45	81.003	-18.168	9.934	1.00	43.34	B
ATOM	1912	NE2	HIS	B	45	82.117	-17.745	9.365	1.00	40.53	B
ATOM	1913	C	HIS	B	45	82.944	-14.139	11.272	1.00	37.82	B
ATOM	1914	O	HIS	B	45	82.439	-13.968	10.164	1.00	39.67	B
ATOM	1915	N	ASN	B	46	84.235	-13.967	11.539	1.00	40.18	B
ATOM	1916	CA	ASN	B	46	85.230	-13.580	10.544	1.00	38.78	B
ATOM	1917	CB	ASN	B	46	86.372	-12.864	11.260	1.00	38.86	B
ATOM	1918	CG	ASN	B	46	87.287	-12.123	10.314	1.00	38.90	B
ATOM	1919	OD1	ASN	B	46	87.647	-12.626	9.248	1.00	39.63	B
ATOM	1920	ND2	ASN	B	46	87.684	-10.923	10.706	1.00	26.83	B
ATOM	1921	C	ASN	B	46	85.719	-14.915	9.969	1.00	39.92	B
ATOM	1922	O	ASN	B	46	85.884	-15.875	10.715	1.00	40.20	B
ATOM	1923	N	ASP	B	47	85.943	-15.007	8.665	1.00	42.60	B



ATOM	1924	CA	ASP	B	47	86.397	-16.288	8.109	1.00	45.88	B
ATOM	1925	CB	ASP	B	47	85.789	-16.522	6.712	1.00	43.41	B
ATOM	1926	CG	ASP	B	47	84.333	-17.003	6.768	1.00	46.32	B
ATOM	1927	OD1	ASP	B	47	84.062	-18.030	7.430	1.00	48.27	B
ATOM	1928	OD2	ASP	B	47	83.452	-16.363	6.143	1.00	46.10	B
ATOM	1929	C	ASP	B	47	87.927	-16.396	8.050	1.00	46.45	B
ATOM	1930	O	ASP	B	47	88.492	-17.491	8.051	1.00	43.03	B
ATOM	1931	N	TYR	B	48	88.595	-15.252	8.001	1.00	47.00	B
ATOM	1932	CA	TYR	B	48	90.044	-15.233	7.954	1.00	48.77	B
ATOM	1933	CB	TYR	B	48	90.527	-14.981	6.528	1.00	49.76	B
ATOM	1934	CG	TYR	B	48	89.944	-15.952	5.520	1.00	56.72	B
ATOM	1935	CD1	TYR	B	48	88.788	-15.629	4.804	1.00	60.39	B
ATOM	1936	CE1	TYR	B	48	88.223	-16.525	3.898	1.00	62.58	B
ATOM	1937	CD2	TYR	B	48	90.527	-17.204	5.301	1.00	58.09	B
ATOM	1938	CE2	TYR	B	48	89.967	-18.114	4.393	1.00	61.62	B
ATOM	1939	CZ	TYR	B	48	88.813	-17.764	3.701	1.00	61.55	B
ATOM	1940	OH	TYR	B	48	88.220	-18.658	2.842	1.00	60.24	B
ATOM	1941	C	TYR	B	48	90.542	-14.149	8.896	1.00	48.73	B
ATOM	1942	O	TYR	B	48	91.113	-13.144	8.465	1.00	49.92	B
ATOM	1943	N	PRO	B	49	90.328	-14.351	10.207	1.00	47.96	B
ATOM	1944	CD	PRO	B	49	89.711	-15.557	10.787	1.00	49.35	B
ATOM	1945	CA	PRO	B	49	90.730	-13.422	11.263	1.00	49.89	B
ATOM	1946	CB	PRO	B	49	90.365	-14.173	12.545	1.00	48.55	B
ATOM	1947	CG	PRO	B	49	90.342	-15.604	12.140	1.00	48.17	B
ATOM	1948	C	PRO	B	49	92.189	-12.973	11.234	1.00	54.32	B
ATOM	1949	O	PRO	B	49	92.461	-11.773	11.151	1.00	55.67	B
ATOM	1950	N	GLU	B	50	93.116	-13.932	11.283	1.00	55.77	B
ATOM	1951	CA	GLU	B	50	94.560	-13.647	11.281	1.00	54.39	B
ATOM	1952	CB	GLU	B	50	95.366	-14.937	11.142	1.00	45.75	B
ATOM	1953	CG	GLU	B	50	94.999	-16.029	12.112	1.00	54.03	B
ATOM	1954	CD	GLU	B	50	93.702	-16.722	11.739	1.00	62.75	B
ATOM	1955	OE1	GLU	B	50	93.232	-16.533	10.590	1.00	65.60	B
ATOM	1956	OE2	GLU	B	50	93.162	-17.467	12.587	1.00	62.82	B
ATOM	1957	C	GLU	B	50	95.095	-12.660	10.236	1.00	53.74	B
ATOM	1958	O	GLU	B	50	96.167	-12.091	10.431	1.00	58.26	B
ATOM	1959	N	THR	B	51	94.382	-12.446	9.138	1.00	49.22	B
ATOM	1960	CA	THR	B	51	94.895	-11.538	8.117	1.00	53.24	B
ATOM	1961	CB	THR	B	51	95.405	-12.336	6.885	1.00	53.66	B
ATOM	1962	OG1	THR	B	51	94.321	-12.620	5.986	1.00	51.32	B
ATOM	1963	CG2	THR	B	51	95.984	-13.657	7.345	1.00	55.70	B
ATOM	1964	C	THR	B	51	93.853	-10.520	7.666	1.00	57.36	B
ATOM	1965	O	THR	B	51	94.171	-9.543	6.970	1.00	58.22	B
ATOM	1966	N	ILE	B	52	92.602	-10.740	8.060	1.00	54.96	B
ATOM	1967	CA	ILE	B	52	91.558	-9.819	7.670	1.00	49.83	B
ATOM	1968	CB	ILE	B	52	90.647	-10.447	6.619	1.00	53.14	B
ATOM	1969	CG2	ILE	B	52	89.506	-9.484	6.275	1.00	54.22	B
ATOM	1970	CG1	ILE	B	52	91.469	-10.797	5.370	1.00	51.52	B
ATOM	1971	CD1	ILE	B	52	90.671	-11.461	4.269	1.00	46.67	B
ATOM	1972	C	ILE	B	52	90.725	-9.400	8.850	1.00	49.01	B
ATOM	1973	O	ILE	B	52	90.384	-10.218	9.700	1.00	47.53	B
ATOM	1974	N	THR	B	53	90.424	-8.107	8.914	1.00	50.04	B
ATOM	1975	CA	THR	B	53	89.591	-7.574	9.982	1.00	51.37	B
ATOM	1976	CB	THR	B	53	90.272	-6.389	10.703	1.00	52.94	B
ATOM	1977	OG1	THR	B	53	91.205	-6.892	11.669	1.00	51.12	B
ATOM	1978	CG2	THR	B	53	89.238	-5.524	11.415	1.00	50.40	B
ATOM	1979	C	THR	B	53	88.265	-7.121	9.384	1.00	50.19	B
ATOM	1980	O	THR	B	53	88.235	-6.305	8.452	1.00	48.62	B
ATOM	1981	N	ASP	B	54	87.175	-7.666	9.923	1.00	49.64	B



ATOM	1982	CA	ASP	B	54	85.836	-7.340	9.443	1.00	48.74	B
ATOM	1983	CB	ASP	B	54	84.953	-8.602	9.442	1.00	47.27	B
ATOM	1984	CG	ASP	B	54	85.315	-9.582	8.320	1.00	44.64	B
ATOM	1985	OD1	ASP	B	54	85.571	-9.119	7.190	1.00	46.93	B
ATOM	1986	OD2	ASP	B	54	85.328	-10.811	8.560	1.00	39.85	B
ATOM	1987	C	ASP	B	54	85.149	-6.226	10.237	1.00	46.99	B
ATOM	1988	O	ASP	B	54	85.266	-6.157	11.460	1.00	41.92	B
ATOM	1989	N	TYR	B	55	84.436	-5.365	9.509	1.00	50.33	B
ATOM	1990	CA	TYR	B	55	83.691	-4.231	10.066	1.00	50.27	B
ATOM	1991	CB	TYR	B	55	84.133	-2.928	9.401	1.00	53.07	B
ATOM	1992	CG	TYR	B	55	85.608	-2.644	9.496	1.00	54.63	B
ATOM	1993	CD1	TYR	B	55	86.317	-2.226	8.366	1.00	51.51	B
ATOM	1994	CE1	TYR	B	55	87.678	-1.991	8.416	1.00	52.19	B
ATOM	1995	CD2	TYR	B	55	86.303	-2.815	10.700	1.00	52.89	B
ATOM	1996	CE2	TYR	B	55	87.678	-2.578	10.767	1.00	58.41	B
ATOM	1997	CZ	TYR	B	55	88.360	-2.168	9.611	1.00	56.38	B
ATOM	1998	OH	TYR	B	55	89.721	-1.953	9.631	1.00	46.61	B
ATOM	1999	C	TYR	B	55	82.189	-4.385	9.835	1.00	47.88	B
ATOM	2000	O	TYR	B	55	81.719	-4.311	8.700	1.00	48.35	B
ATOM	2001	N	VAL	B	56	81.444	-4.577	10.918	1.00	47.78	B
ATOM	2002	CA	VAL	B	56	79.995	-4.728	10.846	1.00	45.91	B
ATOM	2003	CB	VAL	B	56	79.541	-5.895	11.696	1.00	46.70	B
ATOM	2004	CG1	VAL	B	56	78.026	-6.004	11.664	1.00	50.38	B
ATOM	2005	CG2	VAL	B	56	80.179	-7.157	11.169	1.00	47.91	B
ATOM	2006	C	VAL	B	56	79.282	-3.463	11.302	1.00	44.29	B
ATOM	2007	O	VAL	B	56	79.582	-2.905	12.347	1.00	46.32	B
ATOM	2008	N	THR	B	57	78.298	-3.044	10.527	1.00	44.24	B
ATOM	2009	CA	THR	B	57	77.579	-1.810	10.802	1.00	41.17	B
ATOM	2010	CB	THR	B	57	78.069	-0.767	9.784	1.00	35.54	B
ATOM	2011	OG1	THR	B	57	78.063	0.536	10.353	1.00	38.40	B
ATOM	2012	CG2	THR	B	57	77.191	-0.784	8.572	1.00	27.33	B
ATOM	2013	C	THR	B	57	76.054	-1.990	10.654	1.00	41.10	B
ATOM	2014	O	THR	B	57	75.616	-2.869	9.914	1.00	41.91	B
ATOM	2015	N	LEU	B	58	75.252	-1.183	11.357	1.00	39.02	B
ATOM	2016	CA	LEU	B	58	73.798	-1.259	11.199	1.00	39.14	B
ATOM	2017	CB	LEU	B	58	73.052	-0.950	12.501	1.00	38.46	B
ATOM	2018	CG	LEU	B	58	71.522	-0.826	12.309	1.00	38.14	B
ATOM	2019	CD1	LEU	B	58	70.932	-2.186	11.924	1.00	32.30	B
ATOM	2020	CD2	LEU	B	58	70.862	-0.309	13.573	1.00	29.95	B
ATOM	2021	C	LEU	B	58	73.411	-0.219	10.140	1.00	40.92	B
ATOM	2022	O	LEU	B	58	72.990	0.892	10.471	1.00	45.82	B
ATOM	2023	N	GLN	B	59	73.565	-0.604	8.874	1.00	39.41	B
ATOM	2024	CA	GLN	B	59	73.283	0.226	7.702	1.00	39.53	B
ATOM	2025	CB	GLN	B	59	73.319	-0.659	6.450	1.00	45.44	B
ATOM	2026	CG	GLN	B	59	74.135	-0.146	5.275	1.00	54.90	B
ATOM	2027	CD	GLN	B	59	73.755	1.253	4.850	1.00	63.38	B
ATOM	2028	OE1	GLN	B	59	74.192	2.239	5.450	1.00	70.49	B
ATOM	2029	NE2	GLN	B	59	72.930	1.351	3.815	1.00	67.26	B
ATOM	2030	C	GLN	B	59	71.937	0.960	7.747	1.00	38.18	B
ATOM	2031	O	GLN	B	59	71.863	2.156	7.486	1.00	35.51	B
ATOM	2032	N	ARG	B	60	70.877	0.225	8.066	1.00	37.63	B
ATOM	2033	CA	ARG	B	60	69.532	0.780	8.122	1.00	37.38	B
ATOM	2034	CB	ARG	B	60	68.953	0.847	6.704	1.00	38.74	B
ATOM	2035	CG	ARG	B	60	67.663	1.642	6.557	1.00	45.15	B
ATOM	2036	CD	ARG	B	60	67.105	1.553	5.135	1.00	52.51	B
ATOM	2037	NE	ARG	B	60	68.132	1.188	4.152	1.00	69.86	B
ATOM	2038	CZ	ARG	B	60	69.182	1.944	3.816	1.00	74.30	B
ATOM	2039	NH1	ARG	B	60	69.369	3.138	4.377	1.00	74.06	B



ATOM	2040	NH2	ARG	B	60	70.060	1.498	2.920	1.00	73.74	B
ATOM	2041	C	ARG	B	60	68.633	-0.076	9.023	1.00	38.91	B
ATOM	2042	O	ARG	B	60	68.877	-1.265	9.219	1.00	43.16	B
ATOM	2043	N	GLY	B	61	67.603	0.543	9.584	1.00	38.75	B
ATOM	2044	CA	GLY	B	61	66.677	-0.159	10.455	1.00	35.84	B
ATOM	2045	C	GLY	B	61	65.320	0.392	10.099	1.00	36.33	B
ATOM	2046	O	GLY	B	61	65.130	1.603	10.120	1.00	39.54	B
ATOM	2047	N	SER	B	62	64.376	-0.479	9.769	1.00	35.26	B
ATOM	2048	CA	SER	B	62	63.059	-0.022	9.368	1.00	33.15	B
ATOM	2049	CB	SER	B	62	62.901	-0.178	7.861	1.00	36.72	B
ATOM	2050	OG	SER	B	62	63.875	0.585	7.179	1.00	38.32	B
ATOM	2051	C	SER	B	62	61.942	-0.750	10.057	1.00	34.32	B
ATOM	2052	O	SER	B	62	62.029	-1.956	10.287	1.00	39.82	B
ATOM	2053	N	ALA	B	63	60.874	-0.011	10.344	1.00	32.23	B
ATOM	2054	CA	ALA	B	63	59.698	-0.551	11.027	1.00	31.25	B
ATOM	2055	CB	ALA	B	63	59.216	0.433	12.061	1.00	33.63	B
ATOM	2056	C	ALA	B	63	58.559	-0.879	10.073	1.00	27.28	B
ATOM	2057	O	ALA	B	63	58.427	-0.264	9.030	1.00	26.51	B
ATOM	2058	N	TYR	B	64	57.736	-1.848	10.458	1.00	24.98	B
ATOM	2059	CA	TYR	B	64	56.600	-2.288	9.662	1.00	26.45	B
ATOM	2060	CB	TYR	B	64	56.973	-3.516	8.815	1.00	31.53	B
ATOM	2061	CG	TYR	B	64	58.009	-3.217	7.754	1.00	38.26	B
ATOM	2062	CD1	TYR	B	64	59.376	-3.266	8.043	1.00	39.16	B
ATOM	2063	CE1	TYR	B	64	60.322	-2.877	7.101	1.00	41.44	B
ATOM	2064	CD2	TYR	B	64	57.624	-2.784	6.494	1.00	36.50	B
ATOM	2065	CE2	TYR	B	64	58.555	-2.396	5.553	1.00	38.33	B
ATOM	2066	CZ	TYR	B	64	59.898	-2.437	5.856	1.00	44.74	B
ATOM	2067	OH	TYR	B	64	60.803	-2.007	4.914	1.00	50.52	B
ATOM	2068	C	TYR	B	64	55.389	-2.630	10.519	1.00	26.87	B
ATOM	2069	O	TYR	B	64	55.510	-2.908	11.716	1.00	25.93	B
ATOM	2070	N	GLY	B	65	54.219	-2.611	9.887	1.00	26.40	B
ATOM	2071	CA	GLY	B	65	52.986	-2.924	10.582	1.00	23.18	B
ATOM	2072	C	GLY	B	65	52.833	-2.159	11.877	1.00	27.39	B
ATOM	2073	O	GLY	B	65	53.122	-0.948	11.965	1.00	27.74	B
ATOM	2074	N	GLY	B	66	52.393	-2.880	12.898	1.00	27.45	B
ATOM	2075	CA	GLY	B	66	52.172	-2.272	14.195	1.00	31.18	B
ATOM	2076	C	GLY	B	66	53.348	-1.484	14.709	1.00	29.93	B
ATOM	2077	O	GLY	B	66	53.192	-0.363	15.161	1.00	33.78	B
ATOM	2078	N	VAL	B	67	54.533	-2.062	14.638	1.00	29.31	B
ATOM	2079	CA	VAL	B	67	55.701	-1.365	15.127	1.00	32.04	B
ATOM	2080	CB	VAL	B	67	56.983	-2.082	14.715	1.00	32.94	B
ATOM	2081	CG1	VAL	B	67	58.177	-1.150	14.915	1.00	26.67	B
ATOM	2082	CG2	VAL	B	67	57.149	-3.366	15.535	1.00	25.11	B
ATOM	2083	C	VAL	B	67	55.769	0.052	14.607	1.00	33.57	B
ATOM	2084	O	VAL	B	67	56.147	0.974	15.325	1.00	36.86	B
ATOM	2085	N	LEU	B	68	55.379	0.212	13.356	1.00	35.52	B
ATOM	2086	CA	LEU	B	68	55.417	1.496	12.672	1.00	37.28	B
ATOM	2087	CB	LEU	B	68	55.311	1.226	11.176	1.00	36.92	B
ATOM	2088	CG	LEU	B	68	55.556	2.319	10.151	1.00	30.54	B
ATOM	2089	CD1	LEU	B	68	56.941	2.913	10.330	1.00	25.55	B
ATOM	2090	CD2	LEU	B	68	55.396	1.699	8.770	1.00	26.00	B
ATOM	2091	C	LEU	B	68	54.324	2.480	13.092	1.00	39.67	B
ATOM	2092	O	LEU	B	68	54.537	3.693	13.148	1.00	39.11	B
ATOM	2093	N	SER	B	69	53.152	1.956	13.405	1.00	39.21	B
ATOM	2094	CA	SER	B	69	52.053	2.827	13.760	1.00	39.85	B
ATOM	2095	CB	SER	B	69	50.780	2.328	13.087	1.00	40.31	B
ATOM	2096	OG	SER	B	69	50.503	0.990	13.474	1.00	39.64	B
ATOM	2097	C	SER	B	69	51.785	2.996	15.237	1.00	39.99	B



ATOM	2098	O	SER	B	69	51.223	4.008	15.636	1.00	41.46	B
ATOM	2099	N	ASN	B	70	52.187	2.018	16.046	1.00	38.77	B
ATOM	2100	CA	ASN	B	70	51.928	2.058	17.482	1.00	37.31	B
ATOM	2101	CB	ASN	B	70	51.219	0.772	17.900	1.00	35.02	B
ATOM	2102	CG	ASN	B	70	50.006	0.477	17.030	1.00	41.18	B
ATOM	2103	OD1	ASN	B	70	49.351	1.396	16.548	1.00	43.55	B
ATOM	2104	ND2	ASN	B	70	49.697	-0.802	16.830	1.00	42.73	B
ATOM	2105	C	ASN	B	70	53.110	2.286	18.412	1.00	40.36	B
ATOM	2106	O	ASN	B	70	52.940	2.321	19.637	1.00	44.23	B
ATOM	2107	N	PHE	B	71	54.303	2.460	17.865	1.00	37.12	B
ATOM	2108	CA	PHE	B	71	55.438	2.624	18.747	1.00	35.59	B
ATOM	2109	CB	PHE	B	71	56.255	1.328	18.809	1.00	26.81	B
ATOM	2110	CG	PHE	B	71	55.520	0.159	19.394	1.00	21.77	B
ATOM	2111	CD1	PHE	B	71	54.585	-0.537	18.640	1.00	25.54	B
ATOM	2112	CD2	PHE	B	71	55.771	-0.258	20.711	1.00	15.37	B
ATOM	2113	CE1	PHE	B	71	53.891	-1.658	19.198	1.00	35.13	B
ATOM	2114	CE2	PHE	B	71	55.101	-1.356	21.275	1.00	15.51	B
ATOM	2115	CZ	PHE	B	71	54.158	-2.064	20.524	1.00	21.20	B
ATOM	2116	C	PHE	B	71	56.371	3.745	18.359	1.00	38.87	B
ATOM	2117	O	PHE	B	71	56.329	4.259	17.235	1.00	38.70	B
ATOM	2118	N	SER	B	72	57.197	4.131	19.325	1.00	37.57	B
ATOM	2119	CA	SER	B	72	58.223	5.143	19.126	1.00	42.10	B
ATOM	2120	CB	SER	B	72	57.927	6.426	19.911	1.00	44.92	B
ATOM	2121	OG	SER	B	72	57.983	6.205	21.309	1.00	52.03	B
ATOM	2122	C	SER	B	72	59.403	4.408	19.732	1.00	42.52	B
ATOM	2123	O	SER	B	72	59.264	3.746	20.764	1.00	42.31	B
ATOM	2124	N	GLY	B	73	60.563	4.476	19.110	1.00	42.63	B
ATOM	2125	CA	GLY	B	73	61.629	3.717	19.717	1.00	45.46	B
ATOM	2126	C	GLY	B	73	63.039	3.995	19.301	1.00	43.22	B
ATOM	2127	O	GLY	B	73	63.311	4.815	18.414	1.00	40.98	B
ATOM	2128	N	THR	B	74	63.942	3.289	19.967	1.00	40.40	B
ATOM	2129	CA	THR	B	74	65.349	3.446	19.680	1.00	44.94	B
ATOM	2130	CB	THR	B	74	66.135	4.058	20.884	1.00	45.16	B
ATOM	2131	OG1	THR	B	74	66.173	3.116	21.965	1.00	49.01	B
ATOM	2132	CG2	THR	B	74	65.482	5.355	21.353	1.00	36.56	B
ATOM	2133	C	THR	B	74	65.945	2.101	19.363	1.00	42.78	B
ATOM	2134	O	THR	B	74	65.336	1.056	19.615	1.00	36.90	B
ATOM	2135	N	VAL	B	75	67.138	2.146	18.783	1.00	45.54	B
ATOM	2136	CA	VAL	B	75	67.875	0.936	18.455	1.00	45.23	B
ATOM	2137	CB	VAL	B	75	68.138	0.786	16.915	1.00	46.50	B
ATOM	2138	CG1	VAL	B	75	68.889	2.013	16.355	1.00	40.23	B
ATOM	2139	CG2	VAL	B	75	68.919	-0.483	16.657	1.00	36.18	B
ATOM	2140	C	VAL	B	75	69.194	1.045	19.189	1.00	43.29	B
ATOM	2141	O	VAL	B	75	69.909	2.041	19.055	1.00	38.99	B
ATOM	2142	N	LYS	B	76	69.489	0.040	20.000	1.00	45.21	B
ATOM	2143	CA	LYS	B	76	70.743	0.029	20.732	1.00	49.90	B
ATOM	2144	CB	LYS	B	76	70.545	-0.495	22.159	1.00	53.90	B
ATOM	2145	CG	LYS	B	76	71.714	-0.162	23.084	1.00	60.28	B
ATOM	2146	CD	LYS	B	76	71.479	-0.629	24.516	1.00	64.78	B
ATOM	2147	CE	LYS	B	76	72.622	-0.184	25.431	1.00	67.77	B
ATOM	2148	NZ	LYS	B	76	72.421	-0.608	26.851	1.00	72.80	B
ATOM	2149	C	LYS	B	76	71.741	-0.863	19.993	1.00	50.41	B
ATOM	2150	O	LYS	B	76	71.620	-2.091	20.011	1.00	50.36	B
ATOM	2151	N	TYR	B	77	72.717	-0.238	19.339	1.00	48.10	B
ATOM	2152	CA	TYR	B	77	73.734	-0.978	18.606	1.00	47.37	B
ATOM	2153	CB	TYR	B	77	73.890	-0.451	17.188	1.00	40.25	B
ATOM	2154	CG	TYR	B	77	74.855	-1.288	16.379	1.00	42.46	B
ATOM	2155	CD1	TYR	B	77	74.661	-2.660	16.245	1.00	40.68	B



ATOM	2156	CE1	TYR	B	77	75.502	-3.431	15.462	1.00	44.37	B
ATOM	2157	CD2	TYR	B	77	75.932	-0.709	15.712	1.00	44.07	B
ATOM	2158	CE2	TYR	B	77	76.787	-1.467	14.919	1.00	39.44	B
ATOM	2159	CZ	TYR	B	77	76.564	-2.833	14.789	1.00	48.45	B
ATOM	2160	OH	TYR	B	77	77.347	-3.604	13.936	1.00	48.36	B
ATOM	2161	C	TYR	B	77	75.108	-0.930	19.242	1.00	50.29	B
ATOM	2162	O	TYR	B	77	75.811	0.070	19.116	1.00	52.49	B
ATOM	2163	N	SER	B	78	75.503	-2.008	19.906	1.00	51.15	B
ATOM	2164	CA	SER	B	78	76.827	-2.059	20.504	1.00	53.96	B
ATOM	2165	CB	SER	B	78	77.892	-1.901	19.398	1.00	52.80	B
ATOM	2166	OG	SER	B	78	79.223	-2.118	19.863	1.00	45.51	B
ATOM	2167	C	SER	B	78	77.022	-0.986	21.567	1.00	57.66	B
ATOM	2168	O	SER	B	78	77.957	-0.191	21.488	1.00	61.05	B
ATOM	2169	N	GLY	B	79	76.142	-0.947	22.558	1.00	59.91	B
ATOM	2170	CA	GLY	B	79	76.301	0.044	23.609	1.00	60.98	B
ATOM	2171	C	GLY	B	79	75.660	1.407	23.410	1.00	61.44	B
ATOM	2172	O	GLY	B	79	75.304	2.048	24.394	1.00	64.54	B
ATOM	2173	N	SER	B	80	75.521	1.861	22.166	1.00	59.37	B
ATOM	2174	CA	SER	B	80	74.908	3.164	21.888	1.00	58.61	B
ATOM	2175	CB	SER	B	80	75.760	3.946	20.898	1.00	56.52	B
ATOM	2176	OG	SER	B	80	76.995	4.272	21.491	1.00	65.42	B
ATOM	2177	C	SER	B	80	73.480	3.061	21.347	1.00	57.58	B
ATOM	2178	O	SER	B	80	73.070	2.007	20.851	1.00	56.15	B
ATOM	2179	N	SER	B	81	72.724	4.157	21.443	1.00	54.53	B
ATOM	2180	CA	SER	B	81	71.344	4.162	20.963	1.00	49.40	B
ATOM	2181	CB	SER	B	81	70.356	4.417	22.110	1.00	51.39	B
ATOM	2182	OG	SER	B	81	69.796	3.204	22.597	1.00	47.28	B
ATOM	2183	C	SER	B	81	71.102	5.162	19.852	1.00	45.77	B
ATOM	2184	O	SER	B	81	71.765	6.192	19.747	1.00	39.61	B
ATOM	2185	N	TYR	B	82	70.152	4.826	18.996	1.00	45.93	B
ATOM	2186	CA	TYR	B	82	69.830	5.688	17.880	1.00	46.60	B
ATOM	2187	CB	TYR	B	82	70.613	5.268	16.616	1.00	49.73	B
ATOM	2188	CG	TYR	B	82	72.093	5.009	16.838	1.00	51.38	B
ATOM	2189	CD1	TYR	B	82	72.528	3.887	17.552	1.00	49.31	B
ATOM	2190	CE1	TYR	B	82	73.885	3.675	17.818	1.00	53.08	B
ATOM	2191	CD2	TYR	B	82	73.057	5.911	16.383	1.00	55.97	B
ATOM	2192	CE2	TYR	B	82	74.428	5.707	16.639	1.00	54.20	B
ATOM	2193	CZ	TYR	B	82	74.831	4.590	17.360	1.00	56.12	B
ATOM	2194	OH	TYR	B	82	76.171	4.388	17.625	1.00	59.66	B
ATOM	2195	C	TYR	B	82	68.332	5.598	17.611	1.00	44.35	B
ATOM	2196	O	TYR	B	82	67.644	4.643	18.024	1.00	40.57	B
ATOM	2197	N	PRO	B	83	67.807	6.597	16.907	1.00	39.76	B
ATOM	2198	CD	PRO	B	83	68.528	7.801	16.482	1.00	36.79	B
ATOM	2199	CA	PRO	B	83	66.395	6.680	16.553	1.00	39.99	B
ATOM	2200	CB	PRO	B	83	66.306	8.016	15.839	1.00	37.53	B
ATOM	2201	CG	PRO	B	83	67.428	8.795	16.431	1.00	42.77	B
ATOM	2202	C	PRO	B	83	65.984	5.535	15.642	1.00	41.79	B
ATOM	2203	O	PRO	B	83	66.655	5.259	14.656	1.00	46.83	B
ATOM	2204	N	PHE	B	84	64.889	4.868	15.975	1.00	41.27	B
ATOM	2205	CA	PHE	B	84	64.381	3.779	15.146	1.00	41.36	B
ATOM	2206	CB	PHE	B	84	64.508	2.440	15.866	1.00	37.32	B
ATOM	2207	CG	PHE	B	84	63.949	1.288	15.089	1.00	34.18	B
ATOM	2208	CD1	PHE	B	84	64.674	0.710	14.050	1.00	33.03	B
ATOM	2209	CD2	PHE	B	84	62.683	0.789	15.383	1.00	31.71	B
ATOM	2210	CE1	PHE	B	84	64.141	-0.355	13.316	1.00	36.61	B
ATOM	2211	CE2	PHE	B	84	62.139	-0.278	14.655	1.00	31.84	B
ATOM	2212	CZ	PHE	B	84	62.870	-0.852	13.621	1.00	31.68	B
ATOM	2213	C	PHE	B	84	62.905	4.044	14.829	1.00	43.37	B



ATOM	2214	O	PHE	B	84	62.092	4.243	15.744	1.00	46.09	B
ATOM	2215	N	PRO	B	85	62.525	4.016	13.533	1.00	41.86	B
ATOM	2216	CD	PRO	B	85	61.111	4.228	13.179	1.00	35.59	B
ATOM	2217	CA	PRO	B	85	63.328	3.778	12.322	1.00	41.21	B
ATOM	2218	CB	PRO	B	85	62.391	4.235	11.211	1.00	39.09	B
ATOM	2219	CG	PRO	B	85	61.057	3.767	11.740	1.00	33.50	B
ATOM	2220	C	PRO	B	85	64.636	4.543	12.337	1.00	39.65	B
ATOM	2221	O	PRO	B	85	64.690	5.638	12.873	1.00	43.24	B
ATOM	2222	N	THR	B	86	65.683	3.973	11.757	1.00	36.93	B
ATOM	2223	CA	THR	B	86	66.984	4.626	11.750	1.00	38.77	B
ATOM	2224	CB	THR	B	86	68.091	3.640	11.422	1.00	36.90	B
ATOM	2225	OG1	THR	B	86	67.971	3.232	10.057	1.00	38.71	B
ATOM	2226	CG2	THR	B	86	68.006	2.424	12.322	1.00	39.15	B
ATOM	2227	C	THR	B	86	67.044	5.752	10.744	1.00	43.31	B
ATOM	2228	O	THR	B	86	66.257	5.794	9.802	1.00	43.75	B
ATOM	2229	N	THR	B	87	67.993	6.658	10.942	1.00	50.06	B
ATOM	2230	CA	THR	B	87	68.152	7.818	10.059	1.00	55.86	B
ATOM	2231	CB	THR	B	87	67.811	9.115	10.800	1.00	54.71	B
ATOM	2232	OG1	THR	B	87	68.378	9.066	12.116	1.00	63.13	B
ATOM	2233	CG2	THR	B	87	66.313	9.294	10.892	1.00	54.15	B
ATOM	2234	C	THR	B	87	69.558	7.975	9.484	1.00	57.39	B
ATOM	2235	O	THR	B	87	69.781	8.808	8.609	1.00	56.92	B
ATOM	2236	N	SER	B	88	70.501	7.177	9.979	1.00	58.59	B
ATOM	2237	CA	SER	B	88	71.878	7.238	9.506	1.00	58.12	B
ATOM	2238	CB	SER	B	88	72.662	8.281	10.304	1.00	58.73	B
ATOM	2239	OG	SER	B	88	72.921	7.819	11.620	1.00	60.37	B
ATOM	2240	C	SER	B	88	72.555	5.887	9.681	1.00	57.61	B
ATOM	2241	O	SER	B	88	72.134	5.078	10.509	1.00	55.11	B
ATOM	2242	N	GLU	B	89	73.602	5.638	8.897	1.00	57.26	B
ATOM	2243	CA	GLU	B	89	74.332	4.388	9.036	1.00	53.85	B
ATOM	2244	CB	GLU	B	89	75.278	4.132	7.857	1.00	56.12	B
ATOM	2245	CG	GLU	B	89	76.360	3.104	8.177	1.00	54.43	B
ATOM	2246	CD	GLU	B	89	76.997	2.504	6.946	1.00	54.39	B
ATOM	2247	OE1	GLU	B	89	77.234	3.236	5.964	1.00	53.88	B
ATOM	2248	OE2	GLU	B	89	77.274	1.293	6.972	1.00	53.17	B
ATOM	2249	C	GLU	B	89	75.130	4.519	10.318	1.00	49.39	B
ATOM	2250	O	GLU	B	89	75.855	5.484	10.526	1.00	48.42	B
ATOM	2251	N	THR	B	90	74.970	3.527	11.171	1.00	47.42	B
ATOM	2252	CA	THR	B	90	75.609	3.463	12.463	1.00	45.32	B
ATOM	2253	CB	THR	B	90	75.028	2.285	13.230	1.00	44.31	B
ATOM	2254	OG1	THR	B	90	74.771	2.685	14.573	1.00	48.38	B
ATOM	2255	CG2	THR	B	90	75.982	1.091	13.196	1.00	33.61	B
ATOM	2256	C	THR	B	90	77.125	3.318	12.400	1.00	47.66	B
ATOM	2257	O	THR	B	90	77.686	3.089	11.335	1.00	46.49	B
ATOM	2258	N	PRO	B	91	77.809	3.490	13.548	1.00	52.88	B
ATOM	2259	CD	PRO	B	91	77.299	4.125	14.779	1.00	52.94	B
ATOM	2260	CA	PRO	B	91	79.272	3.360	13.612	1.00	52.66	B
ATOM	2261	CB	PRO	B	91	79.599	3.858	15.021	1.00	51.12	B
ATOM	2262	CG	PRO	B	91	78.515	4.847	15.290	1.00	49.49	B
ATOM	2263	C	PRO	B	91	79.619	1.880	13.419	1.00	51.26	B
ATOM	2264	O	PRO	B	91	78.761	1.021	13.611	1.00	51.56	B
ATOM	2265	N	ARG	B	92	80.868	1.580	13.069	1.00	52.78	B
ATOM	2266	CA	ARG	B	92	81.275	0.193	12.826	1.00	54.30	B
ATOM	2267	CB	ARG	B	92	82.213	0.126	11.607	1.00	59.45	B
ATOM	2268	CG	ARG	B	92	83.508	0.923	11.716	1.00	66.71	B
ATOM	2269	CD	ARG	B	92	84.424	0.665	10.506	1.00	68.78	B
ATOM	2270	NE	ARG	B	92	85.800	1.161	10.672	1.00	73.17	B
ATOM	2271	CZ	ARG	B	92	86.528	1.045	11.788	1.00	75.02	B



ATOM	2272	NH1	ARG	B	92	86.026	0.460	12.874	1.00	72.41	B
ATOM	2273	NH2	ARG	B	92	87.783	1.482	11.808	1.00	72.05	B
ATOM	2274	C	ARG	B	92	81.897	-0.602	13.972	1.00	50.97	B
ATOM	2275	O	ARG	B	92	82.780	-0.120	14.668	1.00	56.32	B
ATOM	2276	N	VAL	B	93	81.407	-1.826	14.154	1.00	45.19	B
ATOM	2277	CA	VAL	B	93	81.902	-2.756	15.166	1.00	40.21	B
ATOM	2278	CB	VAL	B	93	80.769	-3.566	15.788	1.00	35.96	B
ATOM	2279	CG1	VAL	B	93	81.324	-4.588	16.762	1.00	29.73	B
ATOM	2280	CG2	VAL	B	93	79.810	-2.652	16.479	1.00	43.00	B
ATOM	2281	C	VAL	B	93	82.818	-3.742	14.437	1.00	42.90	B
ATOM	2282	O	VAL	B	93	82.619	-4.008	13.249	1.00	43.72	B
ATOM	2283	N	VAL	B	94	83.817	-4.295	15.125	1.00	43.31	B
ATOM	2284	CA	VAL	B	94	84.707	-5.225	14.439	1.00	42.65	B
ATOM	2285	CB	VAL	B	94	86.228	-4.848	14.547	1.00	41.03	B
ATOM	2286	CG1	VAL	B	94	86.417	-3.333	14.428	1.00	40.89	B
ATOM	2287	CG2	VAL	B	94	86.834	-5.421	15.803	1.00	31.28	B
ATOM	2288	C	VAL	B	94	84.572	-6.659	14.879	1.00	44.53	B
ATOM	2289	O	VAL	B	94	84.361	-6.962	16.058	1.00	41.27	B
ATOM	2290	N	TYR	B	95	84.691	-7.533	13.885	1.00	47.17	B
ATOM	2291	CA	TYR	B	95	84.623	-8.967	14.074	1.00	47.30	B
ATOM	2292	CB	TYR	B	95	83.506	-9.570	13.206	1.00	44.54	B
ATOM	2293	CG	TYR	B	95	82.139	-9.360	13.793	1.00	40.07	B
ATOM	2294	CD1	TYR	B	95	81.574	-8.095	13.838	1.00	36.98	B
ATOM	2295	CE1	TYR	B	95	80.379	-7.876	14.478	1.00	35.11	B
ATOM	2296	CD2	TYR	B	95	81.454	-10.411	14.402	1.00	42.29	B
ATOM	2297	CE2	TYR	B	95	80.250	-10.198	15.050	1.00	41.04	B
ATOM	2298	CZ	TYR	B	95	79.724	-8.924	15.085	1.00	40.92	B
ATOM	2299	OH	TYR	B	95	78.544	-8.686	15.750	1.00	52.81	B
ATOM	2300	C	TYR	B	95	85.983	-9.522	13.665	1.00	46.53	B
ATOM	2301	O	TYR	B	95	86.452	-9.291	12.537	1.00	47.03	B
ATOM	2302	N	ASN	B	96	86.607	-10.241	14.595	1.00	40.40	B
ATOM	2303	CA	ASN	B	96	87.912	-10.836	14.373	1.00	36.00	B
ATOM	2304	CB	ASN	B	96	88.991	-9.949	14.954	1.00	37.54	B
ATOM	2305	CG	ASN	B	96	88.544	-9.275	16.215	1.00	42.61	B
ATOM	2306	OD1	ASN	B	96	88.215	-8.089	16.201	1.00	54.86	B
ATOM	2307	ND2	ASN	B	96	88.500	-10.023	17.314	1.00	37.56	B
ATOM	2308	C	ASN	B	96	88.032	-12.196	15.016	1.00	36.16	B
ATOM	2309	O	ASN	B	96	88.859	-12.408	15.890	1.00	38.38	B
ATOM	2310	N	SER	B	97	87.210	-13.130	14.584	1.00	33.66	B
ATOM	2311	CA	SER	B	97	87.284	-14.463	15.128	1.00	30.79	B
ATOM	2312	CB	SER	B	97	86.908	-14.460	16.600	1.00	16.62	B
ATOM	2313	OG	SER	B	97	86.445	-15.746	16.987	1.00	28.93	B
ATOM	2314	C	SER	B	97	86.359	-15.369	14.339	1.00	34.93	B
ATOM	2315	O	SER	B	97	85.294	-14.949	13.893	1.00	34.96	B
ATOM	2316	N	ARG	B	98	86.791	-16.607	14.138	1.00	38.81	B
ATOM	2317	CA	ARG	B	98	85.989	-17.559	13.407	1.00	40.04	B
ATOM	2318	CB	ARG	B	98	86.818	-18.786	13.016	1.00	43.35	B
ATOM	2319	CG	ARG	B	98	87.890	-18.522	11.967	1.00	53.22	B
ATOM	2320	CD	ARG	B	98	88.492	-19.832	11.428	1.00	61.19	B
ATOM	2321	NE	ARG	B	98	89.443	-19.604	10.336	1.00	69.42	B
ATOM	2322	CZ	ARG	B	98	90.657	-19.071	10.484	1.00	71.95	B
ATOM	2323	NH1	ARG	B	98	91.093	-18.705	11.688	1.00	69.75	B
ATOM	2324	NH2	ARG	B	98	91.435	-18.888	9.421	1.00	72.04	B
ATOM	2325	C	ARG	B	98	84.865	-17.962	14.338	1.00	43.19	B
ATOM	2326	O	ARG	B	98	83.908	-18.616	13.925	1.00	46.97	B
ATOM	2327	N	THR	B	99	84.981	-17.566	15.601	1.00	43.07	B
ATOM	2328	CA	THR	B	99	83.952	-17.896	16.575	1.00	47.92	B
ATOM	2329	CB	THR	B	99	84.472	-17.757	17.998	1.00	46.09	B



ATOM	2330	OG1	THR	B	99	85.720	-18.441	18.117	1.00	51.61	B
ATOM	2331	CG2	THR	B	99	83.483	-18.366	18.966	1.00	46.02	B
ATOM	2332	C	THR	B	99	82.735	-16.981	16.426	1.00	50.30	B
ATOM	2333	O	THR	B	99	82.873	-15.750	16.367	1.00	50.66	B
ATOM	2334	N	ASP	B	100	81.548	-17.584	16.373	1.00	48.39	B
ATOM	2335	CA	ASP	B	100	80.318	-16.818	16.232	1.00	50.11	B
ATOM	2336	CB	ASP	B	100	79.098	-17.731	16.138	1.00	52.94	B
ATOM	2337	CG	ASP	B	100	78.890	-18.305	14.753	1.00	58.51	B
ATOM	2338	OD1	ASP	B	100	79.199	-17.617	13.749	1.00	55.67	B
ATOM	2339	OD2	ASP	B	100	78.387	-19.447	14.676	1.00	61.45	B
ATOM	2340	C	ASP	B	100	80.088	-15.863	17.386	1.00	49.54	B
ATOM	2341	O	ASP	B	100	79.821	-16.281	18.504	1.00	49.52	B
ATOM	2342	N	LYS	B	101	80.190	-14.576	17.090	1.00	51.30	B
ATOM	2343	CA	LYS	B	101	79.964	-13.513	18.055	1.00	49.68	B
ATOM	2344	CB	LYS	B	101	81.015	-12.417	17.872	1.00	52.75	B
ATOM	2345	CG	LYS	B	101	80.670	-11.081	18.506	1.00	59.69	B
ATOM	2346	CD	LYS	B	101	81.785	-10.068	18.294	1.00	58.80	B
ATOM	2347	CE	LYS	B	101	81.469	-8.748	18.963	1.00	60.08	B
ATOM	2348	NZ	LYS	B	101	82.634	-7.847	18.820	1.00	61.72	B
ATOM	2349	C	LYS	B	101	78.570	-12.970	17.737	1.00	47.59	B
ATOM	2350	O	LYS	B	101	78.088	-13.114	16.615	1.00	44.10	B
ATOM	2351	N	PRO	B	102	77.893	-12.359	18.726	1.00	48.05	B
ATOM	2352	CD	PRO	B	102	78.126	-12.429	20.175	1.00	46.67	B
ATOM	2353	CA	PRO	B	102	76.553	-11.823	18.467	1.00	46.05	B
ATOM	2354	CB	PRO	B	102	75.963	-11.650	19.874	1.00	44.50	B
ATOM	2355	CG	PRO	B	102	76.722	-12.638	20.692	1.00	46.71	B
ATOM	2356	C	PRO	B	102	76.614	-10.501	17.723	1.00	40.70	B
ATOM	2357	O	PRO	B	102	77.658	-9.864	17.647	1.00	39.82	B
ATOM	2358	N	TRP	B	103	75.491	-10.117	17.144	1.00	37.30	B
ATOM	2359	CA	TRP	B	103	75.389	-8.843	16.452	1.00	35.99	B
ATOM	2360	CB	TRP	B	103	74.681	-9.064	15.119	1.00	30.34	B
ATOM	2361	CG	TRP	B	103	74.579	-7.851	14.277	1.00	31.38	B
ATOM	2362	CD2	TRP	B	103	73.422	-7.404	13.562	1.00	30.61	B
ATOM	2363	CE2	TRP	B	103	73.783	-6.216	12.886	1.00	23.58	B
ATOM	2364	CE3	TRP	B	103	72.111	-7.889	13.430	1.00	31.21	B
ATOM	2365	CD1	TRP	B	103	75.570	-6.942	14.012	1.00	29.45	B
ATOM	2366	NE1	TRP	B	103	75.097	-5.957	13.176	1.00	26.89	B
ATOM	2367	CZ2	TRP	B	103	72.884	-5.507	12.089	1.00	19.17	B
ATOM	2368	CZ3	TRP	B	103	71.224	-7.178	12.637	1.00	29.96	B
ATOM	2369	CH2	TRP	B	103	71.620	-5.997	11.979	1.00	23.18	B
ATOM	2370	C	TRP	B	103	74.529	-8.073	17.483	1.00	36.03	B
ATOM	2371	O	TRP	B	103	73.307	-8.254	17.575	1.00	35.89	B
ATOM	2372	N	PRO	B	104	75.184	-7.234	18.298	1.00	34.03	B
ATOM	2373	CD	PRO	B	104	76.553	-6.773	17.988	1.00	36.29	B
ATOM	2374	CA	PRO	B	104	74.608	-6.418	19.362	1.00	30.77	B
ATOM	2375	CB	PRO	B	104	75.842	-5.813	20.010	1.00	25.97	B
ATOM	2376	CG	PRO	B	104	76.697	-5.517	18.838	1.00	26.96	B
ATOM	2377	C	PRO	B	104	73.606	-5.375	18.885	1.00	30.38	B
ATOM	2378	O	PRO	B	104	73.921	-4.190	18.755	1.00	30.99	B
ATOM	2379	N	VAL	B	105	72.394	-5.842	18.626	1.00	28.53	B
ATOM	2380	CA	VAL	B	105	71.322	-4.991	18.169	1.00	26.24	B
ATOM	2381	CB	VAL	B	105	70.972	-5.219	16.679	1.00	26.56	B
ATOM	2382	CG1	VAL	B	105	69.944	-4.184	16.231	1.00	23.98	B
ATOM	2383	CG2	VAL	B	105	72.198	-5.112	15.823	1.00	24.94	B
ATOM	2384	C	VAL	B	105	70.098	-5.338	18.978	1.00	28.16	B
ATOM	2385	O	VAL	B	105	69.786	-6.523	19.175	1.00	22.10	B
ATOM	2386	N	ALA	B	106	69.418	-4.302	19.465	1.00	32.05	B
ATOM	2387	CA	ALA	B	106	68.194	-4.499	20.224	1.00	34.01	B



ATOM	2388	CB	ALA	B	106	68.482	-4.598	21.688	1.00	31.60	B
ATOM	2389	C	ALA	B	106	67.265	-3.334	19.952	1.00	38.42	B
ATOM	2390	O	ALA	B	106	67.703	-2.180	19.834	1.00	39.67	B
ATOM	2391	N	LEU	B	107	65.983	-3.666	19.820	1.00	39.39	B
ATOM	2392	CA	LEU	B	107	64.931	-2.695	19.573	1.00	39.55	B
ATOM	2393	CB	LEU	B	107	63.905	-3.276	18.602	1.00	37.52	B
ATOM	2394	CG	LEU	B	107	63.970	-2.848	17.132	1.00	36.22	B
ATOM	2395	CD1	LEU	B	107	65.387	-2.593	16.687	1.00	35.01	B
ATOM	2396	CD2	LEU	B	107	63.319	-3.905	16.296	1.00	27.15	B
ATOM	2397	C	LEU	B	107	64.258	-2.406	20.896	1.00	39.73	B
ATOM	2398	O	LEU	B	107	63.900	-3.327	21.624	1.00	41.16	B
ATOM	2399	N	TYR	B	108	64.132	-1.126	21.221	1.00	42.11	B
ATOM	2400	CA	TYR	B	108	63.462	-0.693	22.445	1.00	43.26	B
ATOM	2401	CB	TYR	B	108	64.375	0.203	23.280	1.00	42.36	B
ATOM	2402	CG	TYR	B	108	65.357	-0.595	24.086	1.00	48.99	B
ATOM	2403	CD1	TYR	B	108	66.634	-0.860	23.601	1.00	58.34	B
ATOM	2404	CE1	TYR	B	108	67.524	-1.667	24.313	1.00	63.83	B
ATOM	2405	CD2	TYR	B	108	64.986	-1.152	25.306	1.00	51.96	B
ATOM	2406	CE2	TYR	B	108	65.858	-1.961	26.027	1.00	59.54	B
ATOM	2407	CZ	TYR	B	108	67.131	-2.219	25.527	1.00	65.06	B
ATOM	2408	OH	TYR	B	108	68.010	-3.027	26.230	1.00	69.27	B
ATOM	2409	C	TYR	B	108	62.224	0.060	21.977	1.00	41.89	B
ATOM	2410	O	TYR	B	108	62.312	1.191	21.492	1.00	41.81	B
ATOM	2411	N	LEU	B	109	61.075	-0.592	22.113	1.00	39.72	B
ATOM	2412	CA	LEU	B	109	59.827	-0.025	21.635	1.00	43.02	B
ATOM	2413	CB	LEU	B	109	59.212	-0.982	20.610	1.00	39.34	B
ATOM	2414	CG	LEU	B	109	60.170	-1.497	19.534	1.00	36.17	B
ATOM	2415	CD1	LEU	B	109	59.463	-2.491	18.626	1.00	31.98	B
ATOM	2416	CD2	LEU	B	109	60.710	-0.334	18.744	1.00	20.51	B
ATOM	2417	C	LEU	B	109	58.804	0.266	22.719	1.00	44.10	B
ATOM	2418	O	LEU	B	109	58.481	-0.617	23.512	1.00	43.98	B
ATOM	2419	N	THR	B	110	58.291	1.500	22.728	1.00	43.50	B
ATOM	2420	CA	THR	B	110	57.282	1.933	23.695	1.00	41.99	B
ATOM	2421	CB	THR	B	110	57.740	3.163	24.481	1.00	44.49	B
ATOM	2422	OG1	THR	B	110	59.001	2.891	25.096	1.00	53.82	B
ATOM	2423	CG2	THR	B	110	56.729	3.503	25.569	1.00	48.58	B
ATOM	2424	C	THR	B	110	55.976	2.288	22.998	1.00	40.09	B
ATOM	2425	O	THR	B	110	55.935	3.168	22.123	1.00	37.35	B
ATOM	2426	N	PRO	B	111	54.883	1.616	23.389	1.00	41.24	B
ATOM	2427	CD	PRO	B	111	54.781	0.584	24.433	1.00	41.65	B
ATOM	2428	CA	PRO	B	111	53.570	1.869	22.789	1.00	43.07	B
ATOM	2429	CB	PRO	B	111	52.651	0.878	23.515	1.00	43.27	B
ATOM	2430	CG	PRO	B	111	53.570	-0.203	23.970	1.00	42.12	B
ATOM	2431	C	PRO	B	111	53.132	3.302	23.005	1.00	41.16	B
ATOM	2432	O	PRO	B	111	53.493	3.927	24.009	1.00	39.11	B
ATOM	2433	N	VAL	B	112	52.367	3.819	22.053	1.00	41.94	B
ATOM	2434	CA	VAL	B	112	51.857	5.176	22.155	1.00	45.88	B
ATOM	2435	CB	VAL	B	112	51.658	5.823	20.767	1.00	47.57	B
ATOM	2436	CG1	VAL	B	112	53.013	6.036	20.097	1.00	43.97	B
ATOM	2437	CG2	VAL	B	112	50.745	4.950	19.907	1.00	36.70	B
ATOM	2438	C	VAL	B	112	50.521	5.112	22.869	1.00	48.87	B
ATOM	2439	O	VAL	B	112	49.854	4.075	22.862	1.00	50.84	B
ATOM	2440	N	SER	B	113	50.134	6.216	23.494	1.00	53.12	B
ATOM	2441	CA	SER	B	113	48.869	6.264	24.221	1.00	55.18	B
ATOM	2442	CB	SER	B	113	48.601	7.685	24.711	1.00	56.10	B
ATOM	2443	OG	SER	B	113	48.456	8.567	23.614	1.00	56.76	B
ATOM	2444	C	SER	B	113	47.696	5.801	23.364	1.00	53.23	B
ATOM	2445	O	SER	B	113	46.718	5.264	23.879	1.00	53.63	B



ATOM	2446	N	SER B 114	47.802	6.003	22.056	1.00	48.75	B
ATOM	2447	CA	SER B 114	46.729	5.628	21.154	1.00	46.92	B
ATOM	2448	CB	SER B 114	46.755	6.538	19.920	1.00	48.64	B
ATOM	2449	OG	SER B 114	47.935	6.362	19.158	1.00	50.05	B
ATOM	2450	C	SER B 114	46.753	4.164	20.731	1.00	46.39	B
ATOM	2451	O	SER B 114	45.871	3.700	20.014	1.00	44.89	B
ATOM	2452	N	ALA B 115	47.757	3.432	21.185	1.00	49.38	B
ATOM	2453	CA	ALA B 115	47.879	2.027	20.834	1.00	53.40	B
ATOM	2454	CB	ALA B 115	49.116	1.443	21.497	1.00	56.78	B
ATOM	2455	C	ALA B 115	46.634	1.216	21.226	1.00	54.70	B
ATOM	2456	O	ALA B 115	46.232	1.197	22.400	1.00	48.97	B
ATOM	2457	N	GLY B 116	46.049	0.533	20.236	1.00	56.98	B
ATOM	2458	CA	GLY B 116	44.853	-0.271	20.461	1.00	57.50	B
ATOM	2459	C	GLY B 116	44.944	-1.354	21.530	1.00	54.48	B
ATOM	2460	O	GLY B 116	45.205	-1.090	22.710	1.00	53.95	B
ATOM	2461	N	GLY B 117	44.677	-2.581	21.113	1.00	50.75	B
ATOM	2462	CA	GLY B 117	44.757	-3.714	22.015	1.00	49.30	B
ATOM	2463	C	GLY B 117	45.923	-4.506	21.459	1.00	45.39	B
ATOM	2464	O	GLY B 117	46.970	-4.621	22.101	1.00	43.18	B
ATOM	2465	N	VAL B 118	45.730	-5.031	20.249	1.00	40.82	B
ATOM	2466	CA	VAL B 118	46.761	-5.775	19.539	1.00	38.09	B
ATOM	2467	CB	VAL B 118	46.141	-6.759	18.560	1.00	36.33	B
ATOM	2468	CG1	VAL B 118	47.195	-7.255	17.577	1.00	27.83	B
ATOM	2469	CG2	VAL B 118	45.525	-7.910	19.331	1.00	33.81	B
ATOM	2470	C	VAL B 118	47.599	-4.782	18.739	1.00	35.91	B
ATOM	2471	O	VAL B 118	47.210	-4.404	17.652	1.00	38.24	B
ATOM	2472	N	ALA B 119	48.739	-4.357	19.272	1.00	32.10	B
ATOM	2473	CA	ALA B 119	49.586	-3.405	18.570	1.00	28.90	B
ATOM	2474	CB	ALA B 119	50.362	-2.597	19.560	1.00	28.57	B
ATOM	2475	C	ALA B 119	50.551	-4.052	17.566	1.00	32.45	B
ATOM	2476	O	ALA B 119	51.188	-3.348	16.789	1.00	33.60	B
ATOM	2477	N	ILE B 120	50.677	-5.379	17.613	1.00	31.08	B
ATOM	2478	CA	ILE B 120	51.532	-6.129	16.703	1.00	30.88	B
ATOM	2479	CB	ILE B 120	52.918	-6.352	17.301	1.00	35.81	B
ATOM	2480	CG2	ILE B 120	53.721	-7.282	16.411	1.00	27.80	B
ATOM	2481	CG1	ILE B 120	53.648	-5.024	17.460	1.00	36.87	B
ATOM	2482	CD1	ILE B 120	54.991	-5.165	18.133	1.00	38.89	B
ATOM	2483	C	ILE B 120	50.914	-7.511	16.418	1.00	35.91	B
ATOM	2484	O	ILE B 120	50.741	-8.321	17.334	1.00	40.23	B
ATOM	2485	N	LYS B 121	50.587	-7.789	15.161	1.00	30.56	B
ATOM	2486	CA	LYS B 121	49.998	-9.073	14.830	1.00	35.75	B
ATOM	2487	CB	LYS B 121	49.273	-9.010	13.473	1.00	44.54	B
ATOM	2488	CG	LYS B 121	47.826	-8.530	13.481	1.00	49.90	B
ATOM	2489	CD	LYS B 121	47.721	-7.060	13.872	1.00	62.79	B
ATOM	2490	CE	LYS B 121	46.366	-6.495	13.487	1.00	65.42	B
ATOM	2491	NZ	LYS B 121	46.120	-6.665	12.020	1.00	68.24	B
ATOM	2492	C	LYS B 121	50.966	-10.266	14.798	1.00	35.90	B
ATOM	2493	O	LYS B 121	52.123	-10.174	14.368	1.00	33.23	B
ATOM	2494	N	ALA B 122	50.458	-11.399	15.261	1.00	34.06	B
ATOM	2495	CA	ALA B 122	51.214	-12.625	15.247	1.00	33.24	B
ATOM	2496	CB	ALA B 122	50.388	-13.749	15.848	1.00	15.20	B
ATOM	2497	C	ALA B 122	51.497	-12.910	13.764	1.00	35.26	B
ATOM	2498	O	ALA B 122	50.585	-12.866	12.931	1.00	35.27	B
ATOM	2499	N	GLY B 123	52.760	-13.180	13.446	1.00	32.76	B
ATOM	2500	CA	GLY B 123	53.136	-13.491	12.081	1.00	33.01	B
ATOM	2501	C	GLY B 123	53.478	-12.307	11.195	1.00	33.84	B
ATOM	2502	O	GLY B 123	53.806	-12.482	10.024	1.00	33.30	B
ATOM	2503	N	SER B 124	53.434	-11.102	11.744	1.00	32.53	B



ATOM	2504	CA	SER B 124	53.704	-9.921	10.937	1.00	32.72	B
ATOM	2505	CB	SER B 124	52.839	-8.745	11.432	1.00	31.20	B
ATOM	2506	OG	SER B 124	53.032	-8.452	12.802	1.00	24.03	B
ATOM	2507	C	SER B 124	55.161	-9.467	10.816	1.00	34.32	B
ATOM	2508	O	SER B 124	56.003	-9.733	11.678	1.00	36.98	B
ATOM	2509	N	LEU B 125	55.451	-8.776	9.723	1.00	32.72	B
ATOM	2510	CA	LEU B 125	56.785	-8.261	9.519	1.00	29.75	B
ATOM	2511	CB	LEU B 125	56.994	-7.753	8.083	1.00	27.40	B
ATOM	2512	CG	LEU B 125	58.322	-7.004	7.913	1.00	27.74	B
ATOM	2513	CD1	LEU B 125	59.482	-7.956	8.153	1.00	20.32	B
ATOM	2514	CD2	LEU B 125	58.402	-6.394	6.539	1.00	26.43	B
ATOM	2515	C	LEU B 125	56.836	-7.108	10.476	1.00	26.95	B
ATOM	2516	O	LEU B 125	56.099	-6.138	10.354	1.00	32.13	B
ATOM	2517	N	ILE B 126	57.718	-7.219	11.437	1.00	29.14	B
ATOM	2518	CA	ILE B 126	57.857	-6.192	12.445	1.00	31.84	B
ATOM	2519	CB	ILE B 126	58.036	-6.876	13.812	1.00	34.18	B
ATOM	2520	CG2	ILE B 126	59.342	-6.498	14.466	1.00	23.70	B
ATOM	2521	CG1	ILE B 126	56.810	-6.606	14.653	1.00	30.98	B
ATOM	2522	CD1	ILE B 126	56.827	-7.374	15.923	1.00	49.29	B
ATOM	2523	C	ILE B 126	58.986	-5.234	12.140	1.00	32.54	B
ATOM	2524	O	ILE B 126	58.887	-4.060	12.462	1.00	31.40	B
ATOM	2525	N	ALA B 127	60.048	-5.730	11.501	1.00	32.48	B
ATOM	2526	CA	ALA B 127	61.197	-4.887	11.169	1.00	30.49	B
ATOM	2527	CB	ALA B 127	61.970	-4.546	12.436	1.00	25.31	B
ATOM	2528	C	ALA B 127	62.156	-5.508	10.159	1.00	27.91	B
ATOM	2529	O	ALA B 127	62.198	-6.727	9.988	1.00	32.60	B
ATOM	2530	N	VAL B 128	62.915	-4.656	9.482	1.00	19.26	B
ATOM	2531	CA	VAL B 128	63.912	-5.126	8.540	1.00	19.14	B
ATOM	2532	CB	VAL B 128	63.572	-4.760	7.071	1.00	14.82	B
ATOM	2533	CG1	VAL B 128	64.768	-5.061	6.178	1.00	14.77	B
ATOM	2534	CG2	VAL B 128	62.386	-5.580	6.577	1.00	13.30	B
ATOM	2535	C	VAL B 128	65.226	-4.446	8.949	1.00	22.98	B
ATOM	2536	O	VAL B 128	65.305	-3.220	9.003	1.00	27.09	B
ATOM	2537	N	LEU B 129	66.246	-5.240	9.255	1.00	21.47	B
ATOM	2538	CA	LEU B 129	67.531	-4.699	9.676	1.00	24.76	B
ATOM	2539	CB	LEU B 129	67.909	-5.233	11.055	1.00	26.80	B
ATOM	2540	CG	LEU B 129	66.928	-4.908	12.184	1.00	33.18	B
ATOM	2541	CD1	LEU B 129	67.450	-5.505	13.458	1.00	28.58	B
ATOM	2542	CD2	LEU B 129	66.759	-3.393	12.341	1.00	30.83	B
ATOM	2543	C	LEU B 129	68.633	-5.046	8.696	1.00	29.03	B
ATOM	2544	O	LEU B 129	68.858	-6.218	8.374	1.00	31.02	B
ATOM	2545	N	ILE B 130	69.335	-4.021	8.229	1.00	27.82	B
ATOM	2546	CA	ILE B 130	70.404	-4.231	7.271	1.00	28.56	B
ATOM	2547	CB	ILE B 130	70.310	-3.256	6.082	1.00	28.77	B
ATOM	2548	CG2	ILE B 130	71.511	-3.443	5.163	1.00	23.87	B
ATOM	2549	CG1	ILE B 130	69.019	-3.525	5.301	1.00	23.15	B
ATOM	2550	CD1	ILE B 130	68.791	-2.534	4.190	1.00	33.95	B
ATOM	2551	C	ILE B 130	71.782	-4.123	7.883	1.00	30.91	B
ATOM	2552	O	ILE B 130	72.198	-3.063	8.366	1.00	31.82	B
ATOM	2553	N	LEU B 131	72.478	-5.253	7.841	1.00	32.57	B
ATOM	2554	CA	LEU B 131	73.817	-5.392	8.363	1.00	29.92	B
ATOM	2555	CB	LEU B 131	73.989	-6.793	8.937	1.00	27.43	B
ATOM	2556	CG	LEU B 131	75.339	-7.075	9.589	1.00	35.23	B
ATOM	2557	CD1	LEU B 131	75.207	-8.278	10.512	1.00	34.72	B
ATOM	2558	CD2	LEU B 131	76.396	-7.297	8.517	1.00	32.03	B
ATOM	2559	C	LEU B 131	74.762	-5.180	7.203	1.00	30.34	B
ATOM	2560	O	LEU B 131	74.672	-5.874	6.205	1.00	31.82	B
ATOM	2561	N	ARG B 132	75.668	-4.216	7.335	1.00	33.58	B



ATOM	2562	CA	ARG	B	132	76.636	-3.918	6.281	1.00	32.72	B
ATOM	2563	CB	ARG	B	132	76.558	-2.450	5.910	1.00	29.90	B
ATOM	2564	CG	ARG	B	132	77.554	-2.020	4.892	1.00	24.57	B
ATOM	2565	CD	ARG	B	132	77.230	-0.618	4.505	1.00	28.98	B
ATOM	2566	NE	ARG	B	132	77.771	-0.263	3.202	1.00	44.88	B
ATOM	2567	CZ	ARG	B	132	77.466	0.863	2.558	1.00	52.26	B
ATOM	2568	NH1	ARG	B	132	76.623	1.738	3.106	1.00	53.41	B
ATOM	2569	NH2	ARG	B	132	77.996	1.118	1.364	1.00	49.10	B
ATOM	2570	C	ARG	B	132	78.041	-4.261	6.749	1.00	34.78	B
ATOM	2571	O	ARG	B	132	78.522	-3.720	7.749	1.00	36.33	B
ATOM	2572	N	GLN	B	133	78.697	-5.154	6.009	1.00	35.46	B
ATOM	2573	CA	GLN	B	133	80.033	-5.627	6.352	1.00	31.37	B
ATOM	2574	CB	GLN	B	133	79.981	-7.127	6.635	1.00	31.04	B
ATOM	2575	CG	GLN	B	133	81.331	-7.809	6.828	1.00	38.48	B
ATOM	2576	CD	GLN	B	133	81.903	-8.404	5.549	1.00	37.23	B
ATOM	2577	OE1	GLN	B	133	81.262	-9.204	4.870	1.00	41.88	B
ATOM	2578	NE2	GLN	B	133	83.121	-8.020	5.225	1.00	38.07	B
ATOM	2579	C	GLN	B	133	81.082	-5.351	5.297	1.00	33.10	B
ATOM	2580	O	GLN	B	133	80.913	-5.684	4.120	1.00	32.79	B
ATOM	2581	N	THR	B	134	82.168	-4.728	5.742	1.00	32.27	B
ATOM	2582	CA	THR	B	134	83.312	-4.405	4.902	1.00	31.08	B
ATOM	2583	CB	THR	B	134	83.485	-2.913	4.787	1.00	28.44	B
ATOM	2584	OG1	THR	B	134	83.318	-2.351	6.092	1.00	43.54	B
ATOM	2585	CG2	THR	B	134	82.477	-2.318	3.827	1.00	17.92	B
ATOM	2586	C	THR	B	134	84.552	-4.973	5.605	1.00	34.91	B
ATOM	2587	O	THR	B	134	84.439	-5.789	6.526	1.00	31.52	B
ATOM	2588	N	ASN	B	135	85.739	-4.553	5.180	1.00	38.08	B
ATOM	2589	CA	ASN	B	135	86.948	-5.058	5.817	1.00	43.90	B
ATOM	2590	CB	ASN	B	135	87.226	-6.490	5.364	1.00	43.43	B
ATOM	2591	CG	ASN	B	135	87.306	-6.602	3.862	1.00	45.83	B
ATOM	2592	OD1	ASN	B	135	87.848	-5.719	3.199	1.00	38.68	B
ATOM	2593	ND2	ASN	B	135	86.764	-7.684	3.313	1.00	47.13	B
ATOM	2594	C	ASN	B	135	88.153	-4.199	5.506	1.00	46.43	B
ATOM	2595	O	ASN	B	135	88.082	-3.278	4.686	1.00	48.60	B
ATOM	2596	N	ASN	B	136	89.261	-4.504	6.174	1.00	47.15	B
ATOM	2597	CA	ASN	B	136	90.512	-3.785	5.954	1.00	49.23	B
ATOM	2598	CB	ASN	B	136	91.279	-3.636	7.257	1.00	49.84	B
ATOM	2599	CG	ASN	B	136	91.594	-4.972	7.899	1.00	53.73	B
ATOM	2600	OD1	ASN	B	136	92.152	-5.029	8.995	1.00	55.74	B
ATOM	2601	ND2	ASN	B	136	91.234	-6.057	7.223	1.00	55.06	B
ATOM	2602	C	ASN	B	136	91.362	-4.584	4.992	1.00	51.02	B
ATOM	2603	O	ASN	B	136	92.576	-4.634	5.137	1.00	50.25	B
ATOM	2604	N	TYR	B	137	90.718	-5.232	4.026	1.00	55.30	B
ATOM	2605	CA	TYR	B	137	91.440	-6.042	3.060	1.00	55.24	B
ATOM	2606	CB	TYR	B	137	91.152	-7.527	3.263	1.00	62.18	B
ATOM	2607	CG	TYR	B	137	91.947	-8.398	2.315	1.00	73.43	B
ATOM	2608	CD1	TYR	B	137	93.341	-8.310	2.258	1.00	71.51	B
ATOM	2609	CE1	TYR	B	137	94.075	-9.093	1.374	1.00	75.13	B
ATOM	2610	CD2	TYR	B	137	91.306	-9.299	1.457	1.00	78.65	B
ATOM	2611	CE2	TYR	B	137	92.037	-10.091	0.567	1.00	77.61	B
ATOM	2612	CZ	TYR	B	137	93.415	-9.980	0.534	1.00	76.38	B
ATOM	2613	OH	TYR	B	137	94.127	-10.755	-0.343	1.00	75.82	B
ATOM	2614	C	TYR	B	137	91.163	-5.680	1.619	1.00	53.40	B
ATOM	2615	O	TYR	B	137	92.084	-5.650	0.819	1.00	58.08	B
ATOM	2616	N	ASN	B	138	89.909	-5.406	1.276	1.00	50.33	B
ATOM	2617	CA	ASN	B	138	89.578	-5.040	-0.099	1.00	48.93	B
ATOM	2618	CB	ASN	B	138	89.458	-6.282	-0.961	1.00	51.42	B
ATOM	2619	CG	ASN	B	138	88.427	-7.245	-0.448	1.00	52.18	B



ATOM	2620	OD1	ASN	B	138	88.288	-8.334	-0.980	1.00	57.78	B
ATOM	2621	ND2	ASN	B	138	87.696	-6.855	0.586	1.00	52.16	B
ATOM	2622	C	ASN	B	138	88.304	-4.228	-0.224	1.00	51.07	B
ATOM	2623	O	ASN	B	138	87.829	-3.656	0.757	1.00	53.81	B
ATOM	2624	N	SER	B	139	87.740	-4.180	-1.427	1.00	51.10	B
ATOM	2625	CA	SER	B	139	86.518	-3.398	-1.642	1.00	51.76	B
ATOM	2626	CB	SER	B	139	86.478	-2.854	-3.080	1.00	51.64	B
ATOM	2627	OG	SER	B	139	86.441	-3.906	-4.029	1.00	59.56	B
ATOM	2628	C	SER	B	139	85.201	-4.124	-1.333	1.00	45.24	B
ATOM	2629	O	SER	B	139	84.141	-3.711	-1.805	1.00	42.38	B
ATOM	2630	N	ASP	B	140	85.272	-5.193	-0.543	1.00	42.97	B
ATOM	2631	CA	ASP	B	140	84.083	-5.957	-0.165	1.00	42.60	B
ATOM	2632	CB	ASP	B	140	84.482	-7.220	0.624	1.00	40.34	B
ATOM	2633	CG	ASP	B	140	84.912	-8.376	-0.284	1.00	41.15	B
ATOM	2634	OD1	ASP	B	140	85.331	-9.441	0.233	1.00	30.91	B
ATOM	2635	OD2	ASP	B	140	84.826	-8.223	-1.524	1.00	34.85	B
ATOM	2636	C	ASP	B	140	83.100	-5.113	0.665	1.00	45.06	B
ATOM	2637	O	ASP	B	140	83.428	-4.609	1.741	1.00	44.68	B
ATOM	2638	N	ASP	B	141	81.888	-4.966	0.149	1.00	45.88	B
ATOM	2639	CA	ASP	B	141	80.838	-4.208	0.819	1.00	42.51	B
ATOM	2640	CB	ASP	B	141	80.690	-2.844	0.152	1.00	47.71	B
ATOM	2641	CG	ASP	B	141	79.889	-1.863	0.984	1.00	52.18	B
ATOM	2642	OD1	ASP	B	141	79.089	-2.289	1.849	1.00	53.12	B
ATOM	2643	OD2	ASP	B	141	80.051	-0.650	0.753	1.00	56.00	B
ATOM	2644	C	ASP	B	141	79.558	-5.027	0.616	1.00	39.58	B
ATOM	2645	O	ASP	B	141	78.849	-4.840	-0.375	1.00	39.26	B
ATOM	2646	N	PHE	B	142	79.272	-5.931	1.546	1.00	32.52	B
ATOM	2647	CA	PHE	B	142	78.107	-6.799	1.429	1.00	33.15	B
ATOM	2648	CB	PHE	B	142	78.520	-8.261	1.648	1.00	33.39	B
ATOM	2649	CG	PHE	B	142	79.576	-8.747	0.694	1.00	36.64	B
ATOM	2650	CD1	PHE	B	142	80.722	-9.387	1.168	1.00	40.51	B
ATOM	2651	CD2	PHE	B	142	79.411	-8.609	-0.682	1.00	33.21	B
ATOM	2652	CE1	PHE	B	142	81.687	-9.890	0.282	1.00	33.95	B
ATOM	2653	CE2	PHE	B	142	80.361	-9.104	-1.564	1.00	31.13	B
ATOM	2654	CZ	PHE	B	142	81.504	-9.749	-1.078	1.00	30.25	B
ATOM	2655	C	PHE	B	142	77.011	-6.445	2.420	1.00	35.53	B
ATOM	2656	O	PHE	B	142	77.270	-5.894	3.495	1.00	38.43	B
ATOM	2657	N	GLN	B	143	75.778	-6.780	2.063	1.00	33.86	B
ATOM	2658	CA	GLN	B	143	74.652	-6.491	2.934	1.00	30.03	B
ATOM	2659	CB	GLN	B	143	73.656	-5.581	2.245	1.00	28.31	B
ATOM	2660	CG	GLN	B	143	74.140	-4.193	1.953	1.00	32.79	B
ATOM	2661	CD	GLN	B	143	72.987	-3.292	1.625	1.00	42.93	B
ATOM	2662	OE1	GLN	B	143	72.083	-3.685	0.886	1.00	44.79	B
ATOM	2663	NE2	GLN	B	143	72.998	-2.075	2.175	1.00	48.07	B
ATOM	2664	C	GLN	B	143	73.934	-7.751	3.351	1.00	29.96	B
ATOM	2665	O	GLN	B	143	73.617	-8.602	2.523	1.00	28.85	B
ATOM	2666	N	PHE	B	144	73.696	-7.865	4.650	1.00	30.75	B
ATOM	2667	CA	PHE	B	144	73.006	-9.002	5.220	1.00	28.73	B
ATOM	2668	CB	PHE	B	144	73.823	-9.602	6.358	1.00	26.51	B
ATOM	2669	CG	PHE	B	144	75.079	-10.278	5.897	1.00	30.21	B
ATOM	2670	CD1	PHE	B	144	76.129	-9.543	5.350	1.00	29.83	B
ATOM	2671	CD2	PHE	B	144	75.215	-11.667	6.004	1.00	34.24	B
ATOM	2672	CE1	PHE	B	144	77.303	-10.187	4.917	1.00	24.03	B
ATOM	2673	CE2	PHE	B	144	76.376	-12.313	5.577	1.00	25.07	B
ATOM	2674	CZ	PHE	B	144	77.420	-11.567	5.034	1.00	22.57	B
ATOM	2675	C	PHE	B	144	71.689	-8.451	5.720	1.00	30.12	B
ATOM	2676	O	PHE	B	144	71.647	-7.697	6.697	1.00	32.53	B
ATOM	2677	N	VAL	B	145	70.611	-8.834	5.043	1.00	26.21	B



ATOM	2678	CA	VAL	B	145	69.298	-8.345	5.391	1.00	24.86	B
ATOM	2679	CB	VAL	B	145	68.484	-8.083	4.119	1.00	27.44	B
ATOM	2680	CG1	VAL	B	145	67.112	-7.586	4.481	1.00	22.84	B
ATOM	2681	CG2	VAL	B	145	69.215	-7.059	3.230	1.00	23.64	B
ATOM	2682	C	VAL	B	145	68.524	-9.268	6.296	1.00	27.22	B
ATOM	2683	O	VAL	B	145	68.301	-10.426	5.964	1.00	33.37	B
ATOM	2684	N	TRP	B	146	68.101	-8.751	7.444	1.00	28.51	B
ATOM	2685	CA	TRP	B	146	67.332	-9.550	8.396	1.00	26.43	B
ATOM	2686	CB	TRP	B	146	67.969	-9.459	9.788	1.00	23.18	B
ATOM	2687	CG	TRP	B	146	69.457	-9.701	9.755	1.00	23.47	B
ATOM	2688	CD2	TRP	B	146	70.124	-10.968	9.730	1.00	19.01	B
ATOM	2689	CE2	TRP	B	146	71.508	-10.712	9.603	1.00	22.45	B
ATOM	2690	CE3	TRP	B	146	69.687	-12.298	9.797	1.00	20.35	B
ATOM	2691	CD1	TRP	B	146	70.433	-8.756	9.648	1.00	24.85	B
ATOM	2692	NE1	TRP	B	146	71.669	-9.352	9.552	1.00	28.21	B
ATOM	2693	CZ2	TRP	B	146	72.462	-11.735	9.546	1.00	19.23	B
ATOM	2694	CZ3	TRP	B	146	70.645	-13.327	9.735	1.00	18.67	B
ATOM	2695	CH2	TRP	B	146	72.012	-13.033	9.612	1.00	14.89	B
ATOM	2696	C	TRP	B	146	65.872	-9.084	8.436	1.00	27.93	B
ATOM	2697	O	TRP	B	146	65.578	-7.915	8.682	1.00	30.75	B
ATOM	2698	N	ASN	B	147	64.957	-10.002	8.157	1.00	25.92	B
ATOM	2699	CA	ASN	B	147	63.535	-9.683	8.176	1.00	23.01	B
ATOM	2700	CB	ASN	B	147	62.825	-10.307	6.961	1.00	21.04	B
ATOM	2701	CG	ASN	B	147	63.425	-9.849	5.632	1.00	25.61	B
ATOM	2702	OD1	ASN	B	147	63.616	-8.654	5.389	1.00	22.73	B
ATOM	2703	ND2	ASN	B	147	63.718	-10.800	4.768	1.00	29.40	B
ATOM	2704	C	ASN	B	147	62.978	-10.225	9.477	1.00	25.03	B
ATOM	2705	O	ASN	B	147	62.851	-11.443	9.653	1.00	27.78	B
ATOM	2706	N	ILE	B	148	62.657	-9.315	10.394	1.00	21.98	B
ATOM	2707	CA	ILE	B	148	62.156	-9.697	11.713	1.00	23.38	B
ATOM	2708	CB	ILE	B	148	62.529	-8.625	12.772	1.00	24.49	B
ATOM	2709	CG2	ILE	B	148	62.482	-9.241	14.163	1.00	20.09	B
ATOM	2710	CG1	ILE	B	148	63.892	-7.990	12.443	1.00	26.37	B
ATOM	2711	CD1	ILE	B	148	65.094	-8.922	12.458	1.00	18.27	B
ATOM	2712	C	ILE	B	148	60.646	-9.892	11.779	1.00	24.19	B
ATOM	2713	O	ILE	B	148	59.894	-8.939	11.623	1.00	31.82	B
ATOM	2714	N	TYR	B	149	60.198	-11.113	12.013	1.00	22.13	B
ATOM	2715	CA	TYR	B	149	58.768	-11.376	12.131	1.00	26.16	B
ATOM	2716	CB	TYR	B	149	58.359	-12.580	11.272	1.00	24.29	B
ATOM	2717	CG	TYR	B	149	58.323	-12.309	9.789	1.00	31.59	B
ATOM	2718	CD1	TYR	B	149	59.506	-12.244	9.036	1.00	29.91	B
ATOM	2719	CE1	TYR	B	149	59.473	-11.967	7.678	1.00	30.53	B
ATOM	2720	CD2	TYR	B	149	57.106	-12.088	9.133	1.00	32.75	B
ATOM	2721	CE2	TYR	B	149	57.063	-11.811	7.772	1.00	30.71	B
ATOM	2722	CZ	TYR	B	149	58.246	-11.753	7.052	1.00	36.24	B
ATOM	2723	OH	TYR	B	149	58.194	-11.491	5.705	1.00	42.36	B
ATOM	2724	C	TYR	B	149	58.400	-11.673	13.589	1.00	30.29	B
ATOM	2725	O	TYR	B	149	59.185	-12.282	14.318	1.00	34.87	B
ATOM	2726	N	ALA	B	150	57.217	-11.245	14.021	1.00	30.88	B
ATOM	2727	CA	ALA	B	150	56.768	-11.529	15.385	1.00	31.72	B
ATOM	2728	CB	ALA	B	150	55.968	-10.399	15.913	1.00	27.66	B
ATOM	2729	C	ALA	B	150	55.917	-12.797	15.351	1.00	32.87	B
ATOM	2730	O	ALA	B	150	55.029	-12.927	14.513	1.00	33.67	B
ATOM	2731	N	ASN	B	151	56.182	-13.725	16.264	1.00	31.00	B
ATOM	2732	CA	ASN	B	151	55.452	-14.984	16.287	1.00	32.71	B
ATOM	2733	CB	ASN	B	151	56.261	-16.066	17.006	1.00	37.45	B
ATOM	2734	CG	ASN	B	151	57.406	-16.598	16.175	1.00	36.34	B
ATOM	2735	OD1	ASN	B	151	57.213	-17.075	15.061	1.00	40.47	B



ATOM	2736	ND2	ASN	B	151	58.605	-16.526	16.721	1.00	39.04	B
ATOM	2737	C	ASN	B	151	54.118	-14.883	16.970	1.00	32.85	B
ATOM	2738	O	ASN	B	151	53.249	-15.732	16.781	1.00	37.18	B
ATOM	2739	N	ASN	B	152	53.950	-13.839	17.763	1.00	31.83	B
ATOM	2740	CA	ASN	B	152	52.725	-13.682	18.519	1.00	31.46	B
ATOM	2741	CB	ASN	B	152	52.974	-14.178	19.931	1.00	31.71	B
ATOM	2742	CG	ASN	B	152	53.989	-13.325	20.663	1.00	33.57	B
ATOM	2743	OD1	ASN	B	152	55.195	-13.400	20.406	1.00	39.77	B
ATOM	2744	ND2	ASN	B	152	53.503	-12.492	21.569	1.00	32.71	B
ATOM	2745	C	ASN	B	152	52.235	-12.244	18.600	1.00	31.23	B
ATOM	2746	O	ASN	B	152	52.977	-11.309	18.274	1.00	21.68	B
ATOM	2747	N	ASP	B	153	50.990	-12.083	19.065	1.00	33.06	B
ATOM	2748	CA	ASP	B	153	50.420	-10.753	19.228	1.00	35.00	B
ATOM	2749	CB	ASP	B	153	48.903	-10.785	19.481	1.00	35.22	B
ATOM	2750	CG	ASP	B	153	48.098	-11.399	18.343	1.00	40.27	B
ATOM	2751	OD1	ASP	B	153	48.541	-11.402	17.176	1.00	42.01	B
ATOM	2752	OD2	ASP	B	153	46.974	-11.859	18.629	1.00	35.56	B
ATOM	2753	C	ASP	B	153	51.030	-10.082	20.455	1.00	35.09	B
ATOM	2754	O	ASP	B	153	51.265	-10.728	21.466	1.00	36.89	B
ATOM	2755	N	VAL	B	154	51.297	-8.789	20.346	1.00	34.31	B
ATOM	2756	CA	VAL	B	154	51.764	-8.002	21.466	1.00	31.02	B
ATOM	2757	CB	VAL	B	154	52.986	-7.195	21.123	1.00	31.01	B
ATOM	2758	CG1	VAL	B	154	53.320	-6.251	22.288	1.00	28.37	B
ATOM	2759	CG2	VAL	B	154	54.121	-8.112	20.836	1.00	38.21	B
ATOM	2760	C	VAL	B	154	50.615	-7.022	21.783	1.00	33.12	B
ATOM	2761	O	VAL	B	154	50.396	-6.032	21.070	1.00	32.38	B
ATOM	2762	N	VAL	B	155	49.871	-7.325	22.836	1.00	33.40	B
ATOM	2763	CA	VAL	B	155	48.756	-6.487	23.269	1.00	33.75	B
ATOM	2764	CB	VAL	B	155	47.671	-7.315	24.026	1.00	33.02	B
ATOM	2765	CG1	VAL	B	155	46.746	-6.387	24.779	1.00	35.87	B
ATOM	2766	CG2	VAL	B	155	46.866	-8.159	23.049	1.00	35.78	B
ATOM	2767	C	VAL	B	155	49.183	-5.362	24.203	1.00	32.16	B
ATOM	2768	O	VAL	B	155	50.005	-5.559	25.098	1.00	31.88	B
ATOM	2769	N	VAL	B	156	48.618	-4.183	23.982	1.00	35.48	B
ATOM	2770	CA	VAL	B	156	48.866	-3.020	24.838	1.00	38.42	B
ATOM	2771	CB	VAL	B	156	49.272	-1.792	24.024	1.00	40.77	B
ATOM	2772	CG1	VAL	B	156	49.178	-0.546	24.898	1.00	35.57	B
ATOM	2773	CG2	VAL	B	156	50.691	-1.976	23.471	1.00	40.94	B
ATOM	2774	C	VAL	B	156	47.523	-2.731	25.502	1.00	38.00	B
ATOM	2775	O	VAL	B	156	46.608	-2.225	24.860	1.00	40.60	B
ATOM	2776	N	PRO	B	157	47.387	-3.046	26.795	1.00	38.40	B
ATOM	2777	CD	PRO	B	157	48.444	-3.501	27.705	1.00	40.01	B
ATOM	2778	CA	PRO	B	157	46.135	-2.824	27.533	1.00	39.19	B
ATOM	2779	CB	PRO	B	157	46.504	-3.192	28.967	1.00	38.60	B
ATOM	2780	CG	PRO	B	157	47.642	-4.173	28.778	1.00	42.51	B
ATOM	2781	C	PRO	B	157	45.595	-1.410	27.428	1.00	35.87	B
ATOM	2782	O	PRO	B	157	46.362	-0.436	27.385	1.00	34.12	B
ATOM	2783	N	THR	B	158	44.273	-1.301	27.359	1.00	33.32	B
ATOM	2784	CA	THR	B	158	43.655	0.013	27.282	1.00	38.28	B
ATOM	2785	CB	THR	B	158	42.204	-0.080	26.822	1.00	42.15	B
ATOM	2786	OG1	THR	B	158	41.587	1.203	26.977	1.00	50.48	B
ATOM	2787	CG2	THR	B	158	41.453	-1.089	27.648	1.00	46.98	B
ATOM	2788	C	THR	B	158	43.705	0.682	28.666	1.00	37.13	B
ATOM	2789	O	THR	B	158	43.429	0.039	29.686	1.00	34.91	B
ATOM	2790	N	GLY	B	159	44.077	1.965	28.690	1.00	35.68	B
ATOM	2791	CA	GLY	B	159	44.171	2.700	29.943	1.00	35.75	B
ATOM	2792	C	GLY	B	159	42.882	3.368	30.418	1.00	37.79	B
ATOM	2793	O	GLY	B	159	41.823	3.254	29.777	1.00	37.36	B



ATOM	2794	N	GLY	B	160	42.951	4.051	31.557	1.00	32.85	B
ATOM	2795	CA	GLY	B	160	41.764	4.714	32.049	1.00	33.30	B
ATOM	2796	C	GLY	B	160	41.701	6.073	31.402	1.00	34.94	B
ATOM	2797	O	GLY	B	160	42.698	6.513	30.841	1.00	35.86	B
ATOM	2798	N	CYS	B	161	40.558	6.749	31.477	1.00	35.19	B
ATOM	2799	CA	CYS	B	161	40.436	8.073	30.875	1.00	37.82	B
ATOM	2800	C	CYS	B	161	40.898	9.209	31.799	1.00	39.91	B
ATOM	2801	O	CYS	B	161	41.193	8.982	32.976	1.00	43.89	B
ATOM	2802	CB	CYS	B	161	39.006	8.286	30.460	1.00	37.49	B
ATOM	2803	SG	CYS	B	161	38.372	6.895	29.480	1.00	44.87	B
ATOM	2804	N	ASP	B	162	40.997	10.426	31.269	1.00	39.46	B
ATOM	2805	CA	ASP	B	162	41.421	11.541	32.102	1.00	44.50	B
ATOM	2806	CB	ASP	B	162	42.589	12.307	31.481	1.00	50.21	B
ATOM	2807	CG	ASP	B	162	43.226	13.285	32.468	1.00	63.52	B
ATOM	2808	OD1	ASP	B	162	43.513	12.877	33.619	1.00	65.05	B
ATOM	2809	OD2	ASP	B	162	43.444	14.462	32.102	1.00	70.61	B
ATOM	2810	C	ASP	B	162	40.257	12.474	32.336	1.00	47.74	B
ATOM	2811	O	ASP	B	162	39.556	12.869	31.406	1.00	49.17	B
ATOM	2812	N	VAL	B	163	40.043	12.810	33.596	1.00	49.77	B
ATOM	2813	CA	VAL	B	163	38.948	13.674	33.959	1.00	55.00	B
ATOM	2814	CB	VAL	B	163	38.235	13.134	35.201	1.00	53.21	B
ATOM	2815	CG1	VAL	B	163	37.114	14.062	35.611	1.00	52.34	B
ATOM	2816	CG2	VAL	B	163	37.688	11.735	34.900	1.00	52.49	B
ATOM	2817	C	VAL	B	163	39.463	15.073	34.196	1.00	62.78	B
ATOM	2818	O	VAL	B	163	39.759	15.472	35.314	1.00	65.20	B
ATOM	2819	N	SER	B	164	39.568	15.809	33.101	1.00	72.64	B
ATOM	2820	CA	SER	B	164	40.044	17.179	33.102	1.00	80.75	B
ATOM	2821	CB	SER	B	164	40.125	17.688	31.656	1.00	84.26	B
ATOM	2822	OG	SER	B	164	40.585	16.673	30.770	1.00	80.59	B
ATOM	2823	C	SER	B	164	39.100	18.067	33.910	1.00	85.96	B
ATOM	2824	O	SER	B	164	37.965	18.331	33.488	1.00	86.73	B
ATOM	2825	N	ALA	B	165	39.576	18.520	35.068	1.00	89.66	B
ATOM	2826	CA	ALA	B	165	38.797	19.393	35.948	1.00	94.00	B
ATOM	2827	CB	ALA	B	165	38.319	18.616	37.168	1.00	91.90	B
ATOM	2828	C	ALA	B	165	39.654	20.582	36.386	1.00	96.86	B
ATOM	2829	O	ALA	B	165	40.808	20.407	36.786	1.00	100.35	B
ATOM	2830	N	ARG	B	166	39.098	21.789	36.306	1.00	97.52	B
ATOM	2831	CA	ARG	B	166	39.838	22.985	36.693	1.00	98.96	B
ATOM	2832	CB	ARG	B	166	38.986	24.221	36.417	1.00	97.48	B
ATOM	2833	CG	ARG	B	166	38.598	24.315	34.949	1.00	96.82	B
ATOM	2834	CD	ARG	B	166	37.840	25.588	34.607	1.00	99.58	B
ATOM	2835	NE	ARG	B	166	37.445	25.608	33.195	1.00	101.53	B
ATOM	2836	CZ	ARG	B	166	36.640	26.515	32.644	1.00	100.65	B
ATOM	2837	NH1	ARG	B	166	36.134	27.494	33.385	1.00	97.72	B
ATOM	2838	NH2	ARG	B	166	36.329	26.434	31.353	1.00	98.46	B
ATOM	2839	C	ARG	B	166	40.307	22.926	38.154	1.00	101.70	B
ATOM	2840	O	ARG	B	166	41.518	22.859	38.396	1.00	104.32	B
ATOM	2841	N	ASP	B	167	39.375	22.949	39.114	1.00	101.24	B
ATOM	2842	CA	ASP	B	167	39.712	22.852	40.549	1.00	101.61	B
ATOM	2843	CB	ASP	B	167	40.814	23.842	40.945	1.00	105.04	B
ATOM	2844	CG	ASP	B	167	41.305	23.632	42.383	1.00	108.69	B
ATOM	2845	OD1	ASP	B	167	42.020	24.515	42.904	1.00	112.47	B
ATOM	2846	OD2	ASP	B	167	40.976	22.586	42.995	1.00	106.87	B
ATOM	2847	C	ASP	B	167	38.527	23.064	41.489	1.00	100.64	B
ATOM	2848	O	ASP	B	167	37.380	22.826	41.115	1.00	103.25	B
ATOM	2849	N	VAL	B	168	38.833	23.502	42.712	1.00	96.28	B
ATOM	2850	CA	VAL	B	168	37.853	23.772	43.762	1.00	91.56	B
ATOM	2851	CB	VAL	B	168	38.570	24.071	45.101	1.00	92.06	B



- ATOM	2852	CG1	VAL	B	168	39.670	25.090	44.878	1.00	93.27	B
ATOM	2853	CG2	VAL	B	168	37.576	24.586	46.130	1.00	91.17	B
ATOM	2854	C	VAL	B	168	36.945	24.947	43.390	1.00	85.88	B
ATOM	2855	O	VAL	B	168	37.229	26.101	43.708	1.00	85.97	B
ATOM	2856	N	THR	B	169	35.846	24.628	42.717	1.00	79.23	B
ATOM	2857	CA	THR	B	169	34.885	25.618	42.267	1.00	77.03	B
ATOM	2858	CB	THR	B	169	33.730	24.955	41.502	1.00	76.80	B
ATOM	2859	OG1	THR	B	169	34.212	24.463	40.249	1.00	80.08	B
ATOM	2860	CG2	THR	B	169	32.612	25.948	41.247	1.00	75.39	B
ATOM	2861	C	THR	B	169	34.286	26.455	43.372	1.00	76.63	B
ATOM	2862	O	THR	B	169	33.756	25.929	44.350	1.00	76.32	B
ATOM	2863	N	VAL	B	170	34.363	27.769	43.195	1.00	77.34	B
ATOM	2864	CA	VAL	B	170	33.804	28.707	44.156	1.00	78.44	B
ATOM	2865	CB	VAL	B	170	34.483	30.099	44.066	1.00	81.17	B
ATOM	2866	CG1	VAL	B	170	33.967	30.995	45.171	1.00	82.29	B
ATOM	2867	CG2	VAL	B	170	35.996	29.961	44.180	1.00	83.39	B
ATOM	2868	C	VAL	B	170	32.317	28.855	43.840	1.00	77.18	B
ATOM	2869	O	VAL	B	170	31.927	29.605	42.948	1.00	71.35	B
ATOM	2870	N	THR	B	171	31.500	28.092	44.558	1.00	81.19	B
ATOM	2871	CA	THR	B	171	30.056	28.122	44.395	1.00	84.05	B
ATOM	2872	CB	THR	B	171	29.391	26.887	45.087	1.00	82.25	B
ATOM	2873	OG1	THR	B	171	27.969	27.043	45.102	1.00	86.37	B
ATOM	2874	CG2	THR	B	171	29.862	26.743	46.512	1.00	79.27	B
ATOM	2875	C	THR	B	171	29.595	29.408	45.063	1.00	87.98	B
ATOM	2876	O	THR	B	171	28.578	29.438	45.755	1.00	92.17	B
ATOM	2877	N	LEU	B	172	30.353	30.476	44.839	1.00	89.17	B
ATOM	2878	CA	LEU	B	172	30.056	31.763	45.446	1.00	92.60	B
ATOM	2879	CB	LEU	B	172	31.237	32.733	45.245	1.00	96.55	B
ATOM	2880	CG	LEU	B	172	31.432	33.924	46.208	1.00	98.54	B
ATOM	2881	CD1	LEU	B	172	32.839	34.495	46.034	1.00	98.01	B
ATOM	2882	CD2	LEU	B	172	30.388	35.004	45.953	1.00	98.92	B
ATOM	2883	C	LEU	B	172	28.753	32.431	45.007	1.00	92.79	B
ATOM	2884	O	LEU	B	172	28.174	33.174	45.792	1.00	94.65	B
ATOM	2885	N	PRO	B	173	28.264	32.175	43.773	1.00	90.85	B
ATOM	2886	CD	PRO	B	173	28.521	31.050	42.860	1.00	88.96	B
ATOM	2887	CA	PRO	B	173	27.008	32.847	43.403	1.00	90.43	B
ATOM	2888	CB	PRO	B	173	26.503	32.015	42.218	1.00	88.69	B
ATOM	2889	CG	PRO	B	173	27.124	30.675	42.445	1.00	89.49	B
ATOM	2890	C	PRO	B	173	26.047	32.844	44.588	1.00	90.40	B
ATOM	2891	O	PRO	B	173	25.250	31.920	44.750	1.00	93.67	B
ATOM	2892	N	ASP	B	174	26.149	33.890	45.408	1.00	86.06	B
ATOM	2893	CA	ASP	B	174	25.366	34.043	46.627	1.00	81.80	B
ATOM	2894	CB	ASP	B	174	25.137	35.525	46.902	1.00	85.92	B
ATOM	2895	CG	ASP	B	174	26.441	36.267	47.139	1.00	88.15	B
ATOM	2896	OD1	ASP	B	174	27.202	36.459	46.164	1.00	86.99	B
ATOM	2897	OD2	ASP	B	174	26.716	36.640	48.303	1.00	94.90	B
ATOM	2898	C	ASP	B	174	24.069	33.256	46.666	1.00	77.31	B
ATOM	2899	O	ASP	B	174	23.344	33.169	45.676	1.00	73.43	B
ATOM	2900	N	TYR	B	175	23.806	32.687	47.837	1.00	74.04	B
ATOM	2901	CA	TYR	B	175	22.662	31.822	48.075	1.00	74.02	B
ATOM	2902	CB	TYR	B	175	21.768	32.337	49.199	1.00	70.97	B
ATOM	2903	CG	TYR	B	175	20.473	31.551	49.222	1.00	68.59	B
ATOM	2904	CD1	TYR	B	175	20.482	30.171	49.416	1.00	65.93	B
ATOM	2905	CE1	TYR	B	175	19.318	29.423	49.306	1.00	66.29	B
ATOM	2906	CD2	TYR	B	175	19.257	32.160	48.928	1.00	67.00	B
ATOM	2907	CE2	TYR	B	175	18.087	31.417	48.819	1.00	65.36	B
ATOM	2908	CZ	TYR	B	175	18.127	30.052	49.008	1.00	63.55	B
ATOM	2909	OH	TYR	B	175	16.975	29.321	48.898	1.00	64.36	B



ATOM	2910	C	TYR	B	175	21.750	31.428	46.917	1.00	75.18	B
ATOM	2911	O	TYR	B	175	21.519	30.243	46.695	1.00	83.24	B
ATOM	2912	N	PRO	B	176	21.183	32.392	46.186	1.00	67.87	B
ATOM	2913	CD	PRO	B	176	20.952	33.833	46.386	1.00	60.03	B
ATOM	2914	CA	PRO	B	176	20.331	31.854	45.120	1.00	62.12	B
ATOM	2915	CB	PRO	B	176	19.365	32.998	44.866	1.00	62.04	B
ATOM	2916	CG	PRO	B	176	20.253	34.208	45.109	1.00	66.57	B
ATOM	2917	C	PRO	B	176	21.062	31.406	43.848	1.00	57.47	B
ATOM	2918	O	PRO	B	176	20.572	30.547	43.108	1.00	52.79	B
ATOM	2919	N	GLY	B	177	22.238	31.987	43.619	1.00	56.05	B
ATOM	2920	CA	GLY	B	177	23.030	31.701	42.429	1.00	57.16	B
ATOM	2921	C	GLY	B	177	23.447	30.275	42.097	1.00	57.68	B
ATOM	2922	O	GLY	B	177	23.498	29.406	42.968	1.00	61.93	B
ATOM	2923	N	SER	B	178	23.767	30.047	40.824	1.00	52.24	B
ATOM	2924	CA	SER	B	178	24.184	28.740	40.354	1.00	48.46	B
ATOM	2925	CB	SER	B	178	22.983	27.979	39.791	1.00	45.43	B
ATOM	2926	OG	SER	B	178	22.709	28.358	38.449	1.00	39.13	B
ATOM	2927	C	SER	B	178	25.237	28.891	39.264	1.00	50.58	B
ATOM	2928	O	SER	B	178	25.073	29.696	38.350	1.00	53.44	B
ATOM	2929	N	VAL	B	179	26.317	28.119	39.349	1.00	51.43	B
ATOM	2930	CA	VAL	B	179	27.360	28.202	38.331	1.00	51.70	B
ATOM	2931	CB	VAL	B	179	28.774	28.442	38.919	1.00	46.82	B
ATOM	2932	CG1	VAL	B	179	28.733	29.466	40.009	1.00	50.97	B
ATOM	2933	CG2	VAL	B	179	29.339	27.141	39.438	1.00	52.80	B
ATOM	2934	C	VAL	B	179	27.461	26.905	37.556	1.00	52.92	B
ATOM	2935	O	VAL	B	179	26.909	25.874	37.957	1.00	51.89	B
ATOM	2936	N	PRO	B	180	28.153	26.951	36.408	1.00	54.24	B
ATOM	2937	CD	PRO	B	180	28.525	28.164	35.661	1.00	49.71	B
ATOM	2938	CA	PRO	B	180	28.346	25.760	35.578	1.00	51.83	B
ATOM	2939	CB	PRO	B	180	28.542	26.340	34.185	1.00	49.00	B
ATOM	2940	CG	PRO	B	180	29.273	27.590	34.475	1.00	51.54	B
ATOM	2941	C	PRO	B	180	29.616	25.135	36.151	1.00	47.16	B
ATOM	2942	O	PRO	B	180	30.450	25.839	36.730	1.00	41.66	B
ATOM	2943	N	ILE	B	181	29.736	23.819	36.032	1.00	47.39	B
ATOM	2944	CA	ILE	B	181	30.892	23.108	36.559	1.00	43.01	B
ATOM	2945	CB	ILE	B	181	30.487	21.975	37.493	1.00	44.32	B
ATOM	2946	CG2	ILE	B	181	31.731	21.348	38.073	1.00	50.39	B
ATOM	2947	CG1	ILE	B	181	29.609	22.510	38.622	1.00	46.67	B
ATOM	2948	CD1	ILE	B	181	29.108	21.449	39.572	1.00	44.10	B
ATOM	2949	C	ILE	B	181	31.714	22.512	35.446	1.00	42.62	B
ATOM	2950	O	ILE	B	181	31.323	21.529	34.795	1.00	35.02	B
ATOM	2951	N	PRO	B	182	32.883	23.104	35.208	1.00	47.08	B
ATOM	2952	CD	PRO	B	182	33.468	24.243	35.932	1.00	46.65	B
ATOM	2953	CA	PRO	B	182	33.782	22.631	34.157	1.00	45.30	B
ATOM	2954	CB	PRO	B	182	34.902	23.665	34.164	1.00	49.60	B
ATOM	2955	CG	PRO	B	182	34.278	24.882	34.860	1.00	48.89	B
ATOM	2956	C	PRO	B	182	34.293	21.259	34.535	1.00	44.84	B
ATOM	2957	O	PRO	B	182	34.974	21.098	35.552	1.00	41.12	B
ATOM	2958	N	LEU	B	183	33.933	20.268	33.732	1.00	46.51	B
ATOM	2959	CA	LEU	B	183	34.382	18.909	33.966	1.00	47.25	B
ATOM	2960	CB	LEU	B	183	33.616	18.268	35.132	1.00	50.90	B
ATOM	2961	CG	LEU	B	183	34.309	17.147	35.926	1.00	47.28	B
ATOM	2962	CD1	LEU	B	183	33.434	16.714	37.089	1.00	46.65	B
ATOM	2963	CD2	LEU	B	183	34.588	15.972	35.019	1.00	52.20	B
ATOM	2964	C	LEU	B	183	34.155	18.124	32.687	1.00	48.27	B
ATOM	2965	O	LEU	B	183	33.021	17.901	32.253	1.00	47.09	B
ATOM	2966	N	THR	B	184	35.260	17.724	32.075	1.00	51.78	B
ATOM	2967	CA	THR	B	184	35.224	16.959	30.840	1.00	50.01	B



ATOM	2968	CB	THR	B	184	35.779	17.784	29.677	1.00	51.81	B
ATOM	2969	OG1	THR	B	184	37.008	18.404	30.086	1.00	54.34	B
ATOM	2970	CG2	THR	B	184	34.777	18.853	29.250	1.00	49.61	B
ATOM	2971	C	THR	B	184	36.089	15.723	31.017	1.00	47.48	B
ATOM	2972	O	THR	B	184	36.862	15.626	31.970	1.00	43.70	B
ATOM	2973	N	VAL	B	185	35.935	14.773	30.106	1.00	45.69	B
ATOM	2974	CA	VAL	B	185	36.720	13.558	30.146	1.00	48.55	B
ATOM	2975	CB	VAL	B	185	35.950	12.367	30.778	1.00	49.34	B
ATOM	2976	CG1	VAL	B	185	35.650	12.659	32.207	1.00	57.28	B
ATOM	2977	CG2	VAL	B	185	34.662	12.091	30.015	1.00	46.09	B
ATOM	2978	C	VAL	B	185	37.078	13.160	28.735	1.00	49.59	B
ATOM	2979	O	VAL	B	185	36.259	13.295	27.815	1.00	47.94	B
ATOM	2980	N	TYR	B	186	38.306	12.687	28.559	1.00	48.79	B
ATOM	2981	CA	TYR	B	186	38.727	12.214	27.256	1.00	50.15	B
ATOM	2982	CB	TYR	B	186	39.636	13.221	26.548	1.00	46.07	B
ATOM	2983	CG	TYR	B	186	40.908	13.508	27.265	1.00	52.19	B
ATOM	2984	CD1	TYR	B	186	42.060	12.759	27.016	1.00	59.11	B
ATOM	2985	CE1	TYR	B	186	43.242	13.008	27.714	1.00	63.38	B
ATOM	2986	CD2	TYR	B	186	40.964	14.515	28.224	1.00	61.62	B
ATOM	2987	CE2	TYR	B	186	42.143	14.777	28.932	1.00	64.92	B
ATOM	2988	CZ	TYR	B	186	43.274	14.019	28.676	1.00	65.08	B
ATOM	2989	OH	TYR	B	186	44.420	14.252	29.404	1.00	69.08	B
ATOM	2990	C	TYR	B	186	39.440	10.912	27.513	1.00	50.49	B
ATOM	2991	O	TYR	B	186	39.945	10.682	28.611	1.00	45.48	B
ATOM	2992	N	CYS	B	187	39.430	10.049	26.504	1.00	54.17	B
ATOM	2993	CA	CYS	B	187	40.071	8.745	26.580	1.00	54.62	B
ATOM	2994	C	CYS	B	187	40.984	8.527	25.375	1.00	54.54	B
ATOM	2995	O	CYS	B	187	40.560	8.708	24.235	1.00	53.13	B
ATOM	2996	CB	CYS	B	187	39.027	7.632	26.571	1.00	52.62	B
ATOM	2997	SG	CYS	B	187	37.670	7.762	27.771	1.00	59.10	B
ATOM	2998	N	ALA	B	188	42.223	8.110	25.626	1.00	54.69	B
ATOM	2999	CA	ALA	B	188	43.167	7.838	24.545	1.00	49.13	B
ATOM	3000	CB	ALA	B	188	44.470	7.327	25.119	1.00	45.83	B
ATOM	3001	C	ALA	B	188	42.550	6.804	23.597	1.00	46.77	B
ATOM	3002	O	ALA	B	188	42.814	6.807	22.397	1.00	50.39	B
ATOM	3003	N	LYS	B	189	41.718	5.930	24.146	1.00	43.31	B
ATOM	3004	CA	LYS	B	189	41.036	4.914	23.364	1.00	46.05	B
ATOM	3005	CB	LYS	B	189	41.491	3.510	23.770	1.00	50.03	B
ATOM	3006	CG	LYS	B	189	42.999	3.271	23.742	1.00	52.69	B
ATOM	3007	CD	LYS	B	189	43.549	3.370	22.335	1.00	57.46	B
ATOM	3008	CE	LYS	B	189	42.898	2.356	21.393	1.00	54.01	B
ATOM	3009	NZ	LYS	B	189	43.295	2.618	19.969	1.00	53.51	B
ATOM	3010	C	LYS	B	189	39.554	5.053	23.682	1.00	49.47	B
ATOM	3011	O	LYS	B	189	39.163	4.994	24.852	1.00	52.75	B
ATOM	3012	N	SER	B	190	38.725	5.243	22.661	1.00	48.58	B
ATOM	3013	CA	SER	B	190	37.296	5.378	22.896	1.00	49.55	B
ATOM	3014	CB	SER	B	190	36.535	5.477	21.582	1.00	50.32	B
ATOM	3015	OG	SER	B	190	35.283	4.812	21.694	1.00	54.81	B
ATOM	3016	C	SER	B	190	36.740	4.208	23.693	1.00	49.68	B
ATOM	3017	O	SER	B	190	37.141	3.061	23.500	1.00	49.83	B
ATOM	3018	N	GLN	B	191	35.799	4.514	24.583	1.00	51.29	B
ATOM	3019	CA	GLN	B	191	35.154	3.504	25.425	1.00	46.32	B
ATOM	3020	CB	GLN	B	191	36.149	2.974	26.447	1.00	41.82	B
ATOM	3021	CG	GLN	B	191	36.807	4.054	27.266	1.00	45.33	B
ATOM	3022	CD	GLN	B	191	37.821	3.492	28.225	1.00	47.37	B
ATOM	3023	OE1	GLN	B	191	37.474	2.729	29.123	1.00	52.60	B
ATOM	3024	NE2	GLN	B	191	39.086	3.857	28.040	1.00	48.36	B
ATOM	3025	C	GLN	B	191	33.939	4.075	26.147	1.00	42.53	B



ATOM	3026	O	GLN	B	191	33.827	5.284	26.340	1.00	39.92	B
ATOM	3027	N	ASN	B	192	33.028	3.200	26.546	1.00	44.09	B
ATOM	3028	CA	ASN	B	192	31.841	3.648	27.250	1.00	45.19	B
ATOM	3029	CB	ASN	B	192	30.755	2.607	27.120	1.00	45.99	B
ATOM	3030	CG	ASN	B	192	30.521	2.221	25.699	1.00	57.85	B
ATOM	3031	OD1	ASN	B	192	30.472	3.084	24.809	1.00	62.51	B
ATOM	3032	ND2	ASN	B	192	30.368	0.920	25.457	1.00	65.53	B
ATOM	3033	C	ASN	B	192	32.090	3.947	28.722	1.00	45.30	B
ATOM	3034	O	ASN	B	192	32.642	3.135	29.469	1.00	50.43	B
ATOM	3035	N	LEU	B	193	31.678	5.133	29.133	1.00	42.79	B
ATOM	3036	CA	LEU	B	193	31.828	5.554	30.507	1.00	37.15	B
ATOM	3037	CB	LEU	B	193	32.700	6.805	30.601	1.00	34.69	B
ATOM	3038	CG	LEU	B	193	34.206	6.672	30.424	1.00	37.96	B
ATOM	3039	CD1	LEU	B	193	34.861	8.018	30.702	1.00	30.55	B
ATOM	3040	CD2	LEU	B	193	34.749	5.602	31.375	1.00	40.54	B
ATOM	3041	C	LEU	B	193	30.471	5.876	31.083	1.00	37.77	B
ATOM	3042	O	LEU	B	193	29.516	6.150	30.367	1.00	36.61	B
ATOM	3043	N	GLY	B	194	30.406	5.845	32.401	1.00	40.46	B
ATOM	3044	CA	GLY	B	194	29.187	6.165	33.102	1.00	37.77	B
ATOM	3045	C	GLY	B	194	29.683	6.755	34.391	1.00	35.59	B
ATOM	3046	O	GLY	B	194	30.837	6.516	34.753	1.00	34.65	B
ATOM	3047	N	TYR	B	195	28.864	7.553	35.065	1.00	34.29	B
ATOM	3048	CA	TYR	B	195	29.291	8.099	36.345	1.00	30.40	B
ATOM	3049	CB	TYR	B	195	29.973	9.447	36.171	1.00	27.44	B
ATOM	3050	CG	TYR	B	195	29.028	10.573	35.877	1.00	40.60	B
ATOM	3051	CD1	TYR	B	195	28.508	10.758	34.594	1.00	39.19	B
ATOM	3052	CE1	TYR	B	195	27.627	11.793	34.330	1.00	41.44	B
ATOM	3053	CD2	TYR	B	195	28.638	11.458	36.891	1.00	39.17	B
ATOM	3054	CE2	TYR	B	195	27.752	12.501	36.635	1.00	40.82	B
ATOM	3055	CZ	TYR	B	195	27.249	12.662	35.352	1.00	41.47	B
ATOM	3056	OH	TYR	B	195	26.360	13.680	35.089	1.00	42.88	B
ATOM	3057	C	TYR	B	195	28.142	8.239	37.323	1.00	30.29	B
ATOM	3058	O	TYR	B	195	26.965	8.170	36.950	1.00	31.61	B
ATOM	3059	N	TYR	B	196	28.492	8.393	38.593	1.00	30.42	B
ATOM	3060	CA	TYR	B	196	27.499	8.587	39.639	1.00	29.74	B
ATOM	3061	CB	TYR	B	196	26.939	7.257	40.169	1.00	33.47	B
ATOM	3062	CG	TYR	B	196	27.906	6.391	40.936	1.00	29.20	B
ATOM	3063	CD1	TYR	B	196	28.388	6.771	42.189	1.00	30.92	B
ATOM	3064	CE1	TYR	B	196	29.263	5.967	42.892	1.00	25.31	B
ATOM	3065	CD2	TYR	B	196	28.327	5.185	40.411	1.00	27.03	B
ATOM	3066	CE2	TYR	B	196	29.200	4.374	41.100	1.00	34.13	B
ATOM	3067	CZ	TYR	B	196	29.664	4.764	42.339	1.00	32.37	B
ATOM	3068	OH	TYR	B	196	30.511	3.919	43.008	1.00	30.94	B
ATOM	3069	C	TYR	B	196	28.136	9.372	40.753	1.00	26.07	B
ATOM	3070	O	TYR	B	196	29.355	9.327	40.942	1.00	22.97	B
ATOM	3071	N	LEU	B	197	27.293	10.121	41.456	1.00	25.71	B
ATOM	3072	CA	LEU	B	197	27.710	10.961	42.566	1.00	22.19	B
ATOM	3073	CB	LEU	B	197	26.854	12.219	42.592	1.00	21.83	B
ATOM	3074	CG	LEU	B	197	26.959	13.042	41.318	1.00	23.28	B
ATOM	3075	CD1	LEU	B	197	26.111	14.287	41.458	1.00	27.40	B
ATOM	3076	CD2	LEU	B	197	28.415	13.415	41.071	1.00	25.75	B
ATOM	3077	C	LEU	B	197	27.578	10.200	43.881	1.00	19.99	B
ATOM	3078	O	LEU	B	197	26.825	9.230	43.995	1.00	19.34	B
ATOM	3079	N	SER	B	198	28.307	10.661	44.879	1.00	18.26	B
ATOM	3080	CA	SER	B	198	28.314	10.010	46.175	1.00	19.64	B
ATOM	3081	CB	SER	B	198	29.369	8.911	46.173	1.00	20.93	B
ATOM	3082	OG	SER	B	198	30.661	9.507	46.033	1.00	23.70	B
ATOM	3083	C	SER	B	198	28.666	11.027	47.252	1.00	21.67	B



ATOM	3084	O	SER	B	198	29.533	11.884	47.065	1.00	15.06	B
ATOM	3085	N	GLY	B	199	28.005	10.901	48.394	1.00	24.20	B
ATOM	3086	CA	GLY	B	199	28.252	11.815	49.485	1.00	22.78	B
ATOM	3087	C	GLY	B	199	27.063	11.890	50.411	1.00	24.70	B
ATOM	3088	O	GLY	B	199	26.008	11.329	50.128	1.00	26.26	B
ATOM	3089	N	THR	B	200	27.239	12.585	51.526	1.00	28.78	B
ATOM	3090	CA	THR	B	200	26.183	12.741	52.517	1.00	31.30	B
ATOM	3091	CB	THR	B	200	26.724	13.391	53.773	1.00	30.61	B
ATOM	3092	OG1	THR	B	200	27.818	12.620	54.248	1.00	29.07	B
ATOM	3093	CG2	THR	B	200	25.666	13.435	54.843	1.00	37.01	B
ATOM	3094	C	THR	B	200	25.057	13.593	51.973	1.00	28.61	B
ATOM	3095	O	THR	B	200	25.282	14.688	51.477	1.00	27.34	B
ATOM	3096	N	THR	B	201	23.841	13.085	52.090	1.00	28.10	B
ATOM	3097	CA	THR	B	201	22.675	13.765	51.560	1.00	30.23	B
ATOM	3098	CB	THR	B	201	21.937	12.796	50.633	1.00	26.26	B
ATOM	3099	OG1	THR	B	201	22.347	13.056	49.289	1.00	30.41	B
ATOM	3100	CG2	THR	B	201	20.437	12.920	50.781	1.00	34.96	B
ATOM	3101	C	THR	B	201	21.746	14.314	52.634	1.00	30.10	B
ATOM	3102	O	THR	B	201	21.719	13.806	53.754	1.00	32.16	B
ATOM	3103	N	ALA	B	202	20.963	15.333	52.294	1.00	26.57	B
ATOM	3104	CA	ALA	B	202	20.082	15.919	53.293	1.00	26.82	B
ATOM	3105	CB	ALA	B	202	20.438	17.397	53.492	1.00	17.25	B
ATOM	3106	C	ALA	B	202	18.606	15.795	52.992	1.00	26.52	B
ATOM	3107	O	ALA	B	202	17.791	16.392	53.691	1.00	28.78	B
ATOM	3108	N	ASP	B	203	18.248	15.018	51.977	1.00	26.44	B
ATOM	3109	CA	ASP	B	203	16.839	14.906	51.593	1.00	23.32	B
ATOM	3110	CB	ASP	B	203	16.564	15.802	50.400	1.00	25.97	B
ATOM	3111	CG	ASP	B	203	17.479	15.509	49.226	1.00	32.36	B
ATOM	3112	OD1	ASP	B	203	16.976	15.347	48.096	1.00	39.58	B
ATOM	3113	OD2	ASP	B	203	18.706	15.443	49.424	1.00	38.65	B
ATOM	3114	C	ASP	B	203	16.423	13.507	51.239	1.00	25.20	B
ATOM	3115	O	ASP	B	203	17.264	12.666	50.946	1.00	31.85	B
ATOM	3116	N	ALA	B	204	15.120	13.257	51.268	1.00	23.17	B
ATOM	3117	CA	ALA	B	204	14.574	11.947	50.948	1.00	22.41	B
ATOM	3118	CB	ALA	B	204	13.111	11.927	51.227	1.00	13.89	B
ATOM	3119	C	ALA	B	204	14.829	11.585	49.483	1.00	29.93	B
ATOM	3120	O	ALA	B	204	14.913	10.405	49.132	1.00	36.73	B
ATOM	3121	N	GLY	B	205	14.950	12.595	48.628	1.00	28.61	B
ATOM	3122	CA	GLY	B	205	15.214	12.334	47.226	1.00	31.44	B
ATOM	3123	C	GLY	B	205	16.695	12.060	47.041	1.00	31.13	B
ATOM	3124	O	GLY	B	205	17.185	11.808	45.941	1.00	29.42	B
ATOM	3125	N	ASN	B	206	17.414	12.136	48.147	1.00	33.30	B
ATOM	3126	CA	ASN	B	206	18.838	11.868	48.161	1.00	35.99	B
ATOM	3127	CB	ASN	B	206	19.057	10.351	48.046	1.00	34.91	B
ATOM	3128	CG	ASN	B	206	20.506	9.950	48.241	1.00	40.27	B
ATOM	3129	OD1	ASN	B	206	21.069	9.219	47.428	1.00	46.66	B
ATOM	3130	ND2	ASN	B	206	21.118	10.424	49.322	1.00	39.62	B
ATOM	3131	C	ASN	B	206	19.639	12.617	47.088	1.00	34.31	B
ATOM	3132	O	ASN	B	206	20.594	12.078	46.537	1.00	32.67	B
ATOM	3133	N	SER	B	207	19.282	13.868	46.814	1.00	35.04	B
ATOM	3134	CA	SER	B	207	20.013	14.619	45.795	1.00	34.71	B
ATOM	3135	CB	SER	B	207	19.179	14.732	44.527	1.00	35.48	B
ATOM	3136	OG	SER	B	207	18.189	15.717	44.697	1.00	39.62	B
ATOM	3137	C	SER	B	207	20.483	16.014	46.188	1.00	29.99	B
ATOM	3138	O	SER	B	207	20.903	16.778	45.331	1.00	33.75	B
ATOM	3139	N	ILE	B	208	20.402	16.352	47.469	1.00	27.75	B
ATOM	3140	CA	ILE	B	208	20.856	17.658	47.966	1.00	26.41	B
ATOM	3141	CB	ILE	B	208	19.725	18.408	48.684	1.00	19.43	B



ATOM	3142	CG2	ILE	B	208	20.202	19.751	49.125	1.00	15.89	B
ATOM	3143	CG1	ILE	B	208	18.545	18.582	47.727	1.00	22.27	B
ATOM	3144	CD1	ILE	B	208	17.268	18.938	48.379	1.00	24.92	B
ATOM	3145	C	ILE	B	208	21.991	17.380	48.938	1.00	31.88	B
ATOM	3146	O	ILE	B	208	21.776	16.879	50.046	1.00	35.04	B
ATOM	3147	N	PHE	B	209	23.208	17.687	48.514	1.00	36.15	B
ATOM	3148	CA	PHE	B	209	24.360	17.400	49.344	1.00	39.16	B
ATOM	3149	CB	PHE	B	209	25.629	17.332	48.483	1.00	36.39	B
ATOM	3150	CG	PHE	B	209	25.646	16.150	47.549	1.00	33.22	B
ATOM	3151	CD1	PHE	B	209	25.014	16.218	46.304	1.00	30.15	B
ATOM	3152	CD2	PHE	B	209	26.193	14.933	47.962	1.00	31.74	B
ATOM	3153	CE1	PHE	B	209	24.914	15.089	45.481	1.00	31.81	B
ATOM	3154	CE2	PHE	B	209	26.101	13.793	47.151	1.00	37.20	B
ATOM	3155	CZ	PHE	B	209	25.455	13.873	45.901	1.00	34.03	B
ATOM	3156	C	PHE	B	209	24.541	18.317	50.523	1.00	42.76	B
ATOM	3157	O	PHE	B	209	24.651	19.530	50.383	1.00	47.02	B
ATOM	3158	N	THR	B	210	24.542	17.691	51.693	1.00	46.95	B
ATOM	3159	CA	THR	B	210	24.697	18.335	52.991	1.00	49.81	B
ATOM	3160	CB	THR	B	210	25.045	17.276	54.045	1.00	50.33	B
ATOM	3161	OG1	THR	B	210	23.877	16.496	54.329	1.00	52.23	B
ATOM	3162	CG2	THR	B	210	25.582	17.916	55.309	1.00	52.39	B
ATOM	3163	C	THR	B	210	25.752	19.424	53.039	1.00	52.19	B
ATOM	3164	O	THR	B	210	26.828	19.282	52.459	1.00	49.93	B
ATOM	3165	N	ASN	B	211	25.437	20.508	53.747	1.00	56.58	B
ATOM	3166	CA	ASN	B	211	26.376	21.610	53.884	1.00	58.40	B
ATOM	3167	CB	ASN	B	211	25.683	22.880	54.368	1.00	60.22	B
ATOM	3168	CG	ASN	B	211	26.656	24.041	54.537	1.00	62.16	B
ATOM	3169	OD1	ASN	B	211	26.264	25.136	54.933	1.00	67.38	B
ATOM	3170	ND2	ASN	B	211	27.928	23.804	54.232	1.00	57.41	B
ATOM	3171	C	ASN	B	211	27.459	21.242	54.872	1.00	58.42	B
ATOM	3172	O	ASN	B	211	27.198	21.008	56.048	1.00	57.03	B
ATOM	3173	N	THR	B	212	28.683	21.202	54.376	1.00	60.52	B
ATOM	3174	CA	THR	B	212	29.831	20.864	55.191	1.00	64.62	B
ATOM	3175	CB	THR	B	212	30.573	19.674	54.577	1.00	61.43	B
ATOM	3176	OG1	THR	B	212	29.848	18.474	54.862	1.00	55.72	B
ATOM	3177	CG2	THR	B	212	31.987	19.578	55.118	1.00	62.96	B
ATOM	3178	C	THR	B	212	30.765	22.065	55.276	1.00	70.20	B
ATOM	3179	O	THR	B	212	31.455	22.395	54.312	1.00	71.19	B
ATOM	3180	N	ALA	B	213	30.780	22.716	56.432	1.00	73.39	B
ATOM	3181	CA	ALA	B	213	31.623	23.882	56.636	1.00	76.16	B
ATOM	3182	CB	ALA	B	213	31.195	25.004	55.696	1.00	69.82	B
ATOM	3183	C	ALA	B	213	31.504	24.334	58.081	1.00	78.85	B
ATOM	3184	O	ALA	B	213	30.491	24.073	58.739	1.00	74.22	B
ATOM	3185	N	SER	B	214	32.537	25.014	58.572	1.00	85.01	B
ATOM	3186	CA	SER	B	214	32.520	25.499	59.943	1.00	90.59	B
ATOM	3187	CB	SER	B	214	33.896	25.327	60.584	1.00	89.01	B
ATOM	3188	OG	SER	B	214	33.814	25.478	61.993	1.00	90.44	B
ATOM	3189	C	SER	B	214	32.074	26.965	60.048	1.00	94.26	B
ATOM	3190	O	SER	B	214	31.036	27.249	60.652	1.00	92.95	B
ATOM	3191	N	PHE	B	215	32.839	27.884	59.454	1.00	97.92	B
ATOM	3192	CA	PHE	B	215	32.507	29.316	59.510	1.00	102.65	B
ATOM	3193	CB	PHE	B	215	33.226	30.099	58.403	1.00	110.99	B
ATOM	3194	CG	PHE	B	215	32.937	31.591	58.424	1.00	120.75	B
ATOM	3195	CD1	PHE	B	215	32.974	32.342	57.247	1.00	124.12	B
ATOM	3196	CD2	PHE	B	215	32.626	32.244	59.621	1.00	122.39	B
ATOM	3197	CE1	PHE	B	215	32.705	33.716	57.259	1.00	124.99	B
ATOM	3198	CE2	PHE	B	215	32.357	33.614	59.644	1.00	124.51	B
ATOM	3199	CZ	PHE	B	215	32.396	34.352	58.461	1.00	125.83	B



ATOM	3200	C	PHE	B	215	31.008	29.612	59.417	1.00101.78	B
ATOM	3201	O	PHE	B	215	30.452	29.729	58.320	1.00 98.40	B
ATOM	3202	N	SER	B	216	30.378	29.766	60.580	1.00102.30	B
ATOM	3203	CA	SER	B	216	28.950	30.043	60.669	1.00102.31	B
ATOM	3204	CB	SER	B	216	28.690	31.550	60.635	1.00104.47	B
ATOM	3205	OG	SER	B	216	27.323	31.825	60.897	1.00107.31	B
ATOM	3206	C	SER	B	216	28.237	29.360	59.511	1.00100.63	B
ATOM	3207	O	SER	B	216	28.033	29.949	58.446	1.00102.98	B
ATOM	3208	N	PRO	B	217	27.848	28.099	59.711	1.00 96.87	B
ATOM	3209	CD	PRO	B	217	27.869	27.384	60.999	1.00 96.34	B
ATOM	3210	CA	PRO	B	217	27.158	27.307	58.694	1.00 93.40	B
ATOM	3211	CB	PRO	B	217	26.965	25.964	59.384	1.00 94.81	B
ATOM	3212	CG	PRO	B	217	26.768	26.368	60.811	1.00 96.22	B
ATOM	3213	C	PRO	B	217	25.840	27.892	58.219	1.00 88.20	B
ATOM	3214	O	PRO	B	217	24.821	27.745	58.889	1.00 86.80	B
ATOM	3215	N	ALA	B	218	25.864	28.559	57.069	1.00 81.43	B
ATOM	3216	CA	ALA	B	218	24.644	29.111	56.517	1.00 77.92	B
ATOM	3217	CB	ALA	B	218	24.885	29.605	55.108	1.00 74.00	B
ATOM	3218	C	ALA	B	218	23.671	27.939	56.503	1.00 76.24	B
ATOM	3219	O	ALA	B	218	23.587	27.206	55.520	1.00 81.49	B
ATOM	3220	N	GLN	B	219	22.944	27.760	57.597	1.00 71.04	B
ATOM	3221	CA	GLN	B	219	22.006	26.654	57.718	1.00 70.90	B
ATOM	3222	CB	GLN	B	219	21.485	26.572	59.146	1.00 73.31	B
ATOM	3223	CG	GLN	B	219	20.490	25.451	59.348	1.00 80.97	B
ATOM	3224	CD	GLN	B	219	19.824	25.516	60.695	1.00 86.76	B
ATOM	3225	OE1	GLN	B	219	18.982	24.679	61.027	1.00 92.84	B
ATOM	3226	NE2	GLN	B	219	20.193	26.519	61.486	1.00 90.33	B
ATOM	3227	C	GLN	B	219	20.806	26.691	56.781	1.00 68.73	B
ATOM	3228	O	GLN	B	219	20.396	27.755	56.326	1.00 68.60	B
ATOM	3229	N	GLY	B	220	20.253	25.513	56.497	1.00 66.84	B
ATOM	3230	CA	GLY	B	220	19.066	25.422	55.658	1.00 65.64	B
ATOM	3231	C	GLY	B	220	19.200	25.250	54.156	1.00 62.93	B
ATOM	3232	O	GLY	B	220	18.197	25.016	53.474	1.00 60.58	B
ATOM	3233	N	VAL	B	221	20.419	25.350	53.634	1.00 59.50	B
ATOM	3234	CA	VAL	B	221	20.611	25.209	52.206	1.00 56.77	B
ATOM	3235	CB	VAL	B	221	21.492	26.346	51.648	1.00 56.11	B
ATOM	3236	CG1	VAL	B	221	21.306	26.455	50.145	1.00 55.39	B
ATOM	3237	CG2	VAL	B	221	21.128	27.644	52.300	1.00 52.54	B
ATOM	3238	C	VAL	B	221	21.190	23.853	51.789	1.00 56.04	B
ATOM	3239	O	VAL	B	221	20.626	22.816	52.117	1.00 55.23	B
ATOM	3240	N	GLY	B	222	22.308	23.863	51.066	1.00 54.20	B
ATOM	3241	CA	GLY	B	222	22.895	22.625	50.584	1.00 49.22	B
ATOM	3242	C	GLY	B	222	23.086	22.689	49.076	1.00 44.37	B
ATOM	3243	O	GLY	B	222	22.327	23.351	48.384	1.00 45.67	B
ATOM	3244	N	VAL	B	223	24.099	21.995	48.571	1.00 39.98	B
ATOM	3245	CA	VAL	B	223	24.433	21.976	47.145	1.00 34.73	B
ATOM	3246	CB	VAL	B	223	25.960	21.887	46.972	1.00 37.08	B
ATOM	3247	CG1	VAL	B	223	26.316	21.712	45.508	1.00 37.73	B
ATOM	3248	CG2	VAL	B	223	26.621	23.129	47.564	1.00 33.20	B
ATOM	3249	C	VAL	B	223	23.799	20.825	46.354	1.00 34.60	B
ATOM	3250	O	VAL	B	223	23.819	19.671	46.790	1.00 35.57	B
ATOM	3251	N	GLN	B	224	23.236	21.141	45.188	1.00 32.64	B
ATOM	3252	CA	GLN	B	224	22.611	20.125	44.334	1.00 31.49	B
ATOM	3253	CB	GLN	B	224	21.103	20.311	44.282	1.00 20.31	B
ATOM	3254	CG	GLN	B	224	20.376	19.195	43.586	1.00 27.39	B
ATOM	3255	CD	GLN	B	224	18.894	19.490	43.414	1.00 32.58	B
ATOM	3256	OE1	GLN	B	224	18.052	18.609	43.538	1.00 38.46	B
ATOM	3257	NE2	GLN	B	224	18.573	20.739	43.118	1.00 37.37	B



ATOM	3258	C	GLN	B	224	23.204	20.270	42.933	1.00	34.63	B
ATOM	3259	O	GLN	B	224	23.372	21.384	42.439	1.00	35.45	B
ATOM	3260	N	LEU	B	225	23.558	19.152	42.306	1.00	32.63	B
ATOM	3261	CA	LEU	B	225	24.152	19.212	40.988	1.00	26.59	B
ATOM	3262	CB	LEU	B	225	25.362	18.295	40.897	1.00	26.01	B
ATOM	3263	CG	LEU	B	225	26.470	18.573	41.909	1.00	28.03	B
ATOM	3264	CD1	LEU	B	225	27.738	17.835	41.509	1.00	28.60	B
ATOM	3265	CD2	LEU	B	225	26.739	20.045	41.970	1.00	29.82	B
ATOM	3266	C	LEU	B	225	23.152	18.860	39.921	1.00	29.18	B
ATOM	3267	O	LEU	B	225	22.297	17.972	40.082	1.00	30.83	B
ATOM	3268	N	THR	B	226	23.284	19.556	38.804	1.00	26.74	B
ATOM	3269	CA	THR	B	226	22.369	19.358	37.714	1.00	26.34	B
ATOM	3270	CB	THR	B	226	21.411	20.570	37.722	1.00	23.75	B
ATOM	3271	OG1	THR	B	226	20.156	20.204	37.154	1.00	31.98	B
ATOM	3272	CG2	THR	B	226	22.018	21.731	36.989	1.00	24.18	B
ATOM	3273	C	THR	B	226	23.157	19.202	36.398	1.00	25.37	B
ATOM	3274	O	THR	B	226	24.279	19.712	36.272	1.00	22.87	B
ATOM	3275	N	ARG	B	227	22.599	18.450	35.451	1.00	25.59	B
ATOM	3276	CA	ARG	B	227	23.239	18.232	34.142	1.00	28.66	B
ATOM	3277	CB	ARG	B	227	23.658	16.742	33.950	1.00	24.62	B
ATOM	3278	CG	ARG	B	227	22.522	15.718	34.034	1.00	21.48	B
ATOM	3279	CD	ARG	B	227	23.019	14.269	33.901	1.00	32.32	B
ATOM	3280	NE	ARG	B	227	22.016	13.390	33.284	1.00	29.36	B
ATOM	3281	CZ	ARG	B	227	21.197	12.582	33.947	1.00	34.78	B
ATOM	3282	NH1	ARG	B	227	21.248	12.513	35.277	1.00	41.37	B
ATOM	3283	NH2	ARG	B	227	20.309	11.854	33.278	1.00	32.97	B
ATOM	3284	C	ARG	B	227	22.229	18.683	33.079	1.00	31.96	B
ATOM	3285	O	ARG	B	227	21.265	17.967	32.747	1.00	26.73	B
ATOM	3286	N	ASN	B	228	22.462	19.890	32.561	1.00	38.41	B
ATOM	3287	CA	ASN	B	228	21.559	20.508	31.589	1.00	41.77	B
ATOM	3288	CB	ASN	B	228	21.654	19.805	30.234	1.00	48.17	B
ATOM	3289	CG	ASN	B	228	22.927	20.151	29.497	1.00	57.26	B
ATOM	3290	OD1	ASN	B	228	23.022	19.949	28.288	1.00	65.08	B
ATOM	3291	ND2	ASN	B	228	23.919	20.675	30.222	1.00	55.65	B
ATOM	3292	C	ASN	B	228	20.118	20.469	32.108	1.00	39.23	B
ATOM	3293	O	ASN	B	228	19.196	20.002	31.430	1.00	36.37	B
ATOM	3294	N	GLY	B	229	19.934	20.930	33.337	1.00	38.13	B
ATOM	3295	CA	GLY	B	229	18.605	20.950	33.908	1.00	41.08	B
ATOM	3296	C	GLY	B	229	18.155	19.725	34.678	1.00	43.59	B
ATOM	3297	O	GLY	B	229	17.287	19.843	35.549	1.00	45.67	B
ATOM	3298	N	THR	B	230	18.711	18.557	34.364	1.00	42.49	B
ATOM	3299	CA	THR	B	230	18.332	17.333	35.056	1.00	38.40	B
ATOM	3300	CB	THR	B	230	18.610	16.113	34.211	1.00	39.37	B
ATOM	3301	OG1	THR	B	230	17.706	16.096	33.109	1.00	40.70	B
ATOM	3302	CG2	THR	B	230	18.431	14.841	35.036	1.00	38.46	B
ATOM	3303	C	THR	B	230	19.100	17.179	36.351	1.00	39.61	B
ATOM	3304	O	THR	B	230	20.323	17.354	36.391	1.00	42.86	B
ATOM	3305	N	ILE	B	231	18.372	16.847	37.409	1.00	34.66	B
ATOM	3306	CA	ILE	B	231	18.968	16.670	38.720	1.00	30.66	B
ATOM	3307	CB	ILE	B	231	17.889	16.703	39.830	1.00	35.84	B
ATOM	3308	CG2	ILE	B	231	18.467	16.211	41.162	1.00	31.79	B
ATOM	3309	CG1	ILE	B	231	17.337	18.118	39.979	1.00	31.34	B
ATOM	3310	CD1	ILE	B	231	16.245	18.219	41.030	1.00	38.78	B
ATOM	3311	C	ILE	B	231	19.690	15.346	38.784	1.00	28.43	B
ATOM	3312	O	ILE	B	231	19.227	14.345	38.238	1.00	28.64	B
ATOM	3313	N	ILE	B	232	20.829	15.341	39.460	1.00	28.29	B
ATOM	3314	CA	ILE	B	232	21.605	14.119	39.598	1.00	26.92	B
ATOM	3315	CB	ILE	B	232	23.052	14.347	39.122	1.00	26.05	B



ATOM	3316	CG2	ILE	B	232	23.856	13.055	39.214	1.00	23.10	B
ATOM	3317	CG1	ILE	B	232	23.048	14.846	37.670	1.00	27.40	B
ATOM	3318	CD1	ILE	B	232	24.387	15.385	37.201	1.00	14.12	B
ATOM	3319	C	ILE	B	232	21.624	13.648	41.053	1.00	29.16	B
ATOM	3320	O	ILE	B	232	22.390	14.157	41.877	1.00	33.06	B
ATOM	3321	N	PRO	B	233	20.744	12.703	41.406	1.00	26.93	B
ATOM	3322	CD	PRO	B	233	19.503	12.296	40.730	1.00	17.70	B
ATOM	3323	CA	PRO	B	233	20.771	12.239	42.800	1.00	27.35	B
ATOM	3324	CB	PRO	B	233	19.422	11.522	42.959	1.00	25.87	B
ATOM	3325	CG	PRO	B	233	19.057	11.133	41.563	1.00	24.73	B
ATOM	3326	C	PRO	B	233	21.967	11.306	42.996	1.00	27.88	B
ATOM	3327	O	PRO	B	233	22.426	10.676	42.043	1.00	31.92	B
ATOM	3328	N	ALA	B	234	22.476	11.237	44.218	1.00	26.36	B
ATOM	3329	CA	ALA	B	234	23.617	10.383	44.547	1.00	23.38	B
ATOM	3330	CB	ALA	B	234	23.908	10.470	46.019	1.00	21.51	B
ATOM	3331	C	ALA	B	234	23.358	8.938	44.178	1.00	23.04	B
ATOM	3332	O	ALA	B	234	22.255	8.442	44.379	1.00	22.78	B
ATOM	3333	N	ASN	B	235	24.375	8.267	43.635	1.00	21.90	B
ATOM	3334	CA	ASN	B	235	24.260	6.859	43.259	1.00	24.10	B
ATOM	3335	CB	ASN	B	235	23.996	6.020	44.508	1.00	22.91	B
ATOM	3336	CG	ASN	B	235	25.033	6.275	45.585	1.00	33.34	B
ATOM	3337	OD1	ASN	B	235	24.726	6.808	46.655	1.00	35.54	B
ATOM	3338	ND2	ASN	B	235	26.278	5.921	45.296	1.00	26.96	B
ATOM	3339	C	ASN	B	235	23.220	6.539	42.191	1.00	27.36	B
ATOM	3340	O	ASN	B	235	22.502	5.541	42.285	1.00	29.41	B
ATOM	3341	N	ASN	B	236	23.149	7.402	41.182	1.00	28.35	B
ATOM	3342	CA	ASN	B	236	22.250	7.252	40.048	1.00	28.60	B
ATOM	3343	CB	ASN	B	236	21.262	8.425	40.002	1.00	40.03	B
ATOM	3344	CG	ASN	B	236	20.472	8.490	38.694	1.00	41.42	B
ATOM	3345	OD1	ASN	B	236	19.769	7.556	38.342	1.00	47.61	B
ATOM	3346	ND2	ASN	B	236	20.593	9.602	37.975	1.00	50.59	B
ATOM	3347	C	ASN	B	236	23.220	7.311	38.873	1.00	31.22	B
ATOM	3348	O	ASN	B	236	23.697	8.383	38.521	1.00	35.01	B
ATOM	3349	N	THR	B	237	23.529	6.172	38.270	1.00	27.12	B
ATOM	3350	CA	THR	B	237	24.497	6.180	37.195	1.00	31.43	B
ATOM	3351	CB	THR	B	237	24.953	4.733	36.841	1.00	38.77	B
ATOM	3352	OG1	THR	B	237	25.264	4.009	38.045	1.00	43.58	B
ATOM	3353	CG2	THR	B	237	26.203	4.778	35.974	1.00	38.34	B
ATOM	3354	C	THR	B	237	24.056	6.899	35.929	1.00	30.75	B
ATOM	3355	O	THR	B	237	23.035	6.578	35.326	1.00	31.22	B
ATOM	3356	N	VAL	B	238	24.842	7.888	35.536	1.00	31.25	B
ATOM	3357	CA	VAL	B	238	24.562	8.642	34.330	1.00	36.89	B
ATOM	3358	CB	VAL	B	238	24.856	10.144	34.504	1.00	42.58	B
ATOM	3359	CG1	VAL	B	238	24.820	10.845	33.145	1.00	38.47	B
ATOM	3360	CG2	VAL	B	238	23.830	10.764	35.427	1.00	49.26	B
ATOM	3361	C	VAL	B	238	25.473	8.108	33.243	1.00	39.39	B
ATOM	3362	O	VAL	B	238	26.703	8.139	33.370	1.00	36.75	B
ATOM	3363	N	SER	B	239	24.861	7.628	32.171	1.00	40.84	B
ATOM	3364	CA	SER	B	239	25.617	7.078	31.067	1.00	41.99	B
ATOM	3365	CB	SER	B	239	24.780	6.074	30.311	1.00	43.25	B
ATOM	3366	OG	SER	B	239	25.514	5.637	29.189	1.00	55.86	B
ATOM	3367	C	SER	B	239	26.109	8.117	30.085	1.00	40.52	B
ATOM	3368	O	SER	B	239	25.321	8.789	29.435	1.00	44.65	B
ATOM	3369	N	LEU	B	240	27.421	8.223	29.965	1.00	38.57	B
ATOM	3370	CA	LEU	B	240	28.047	9.171	29.054	1.00	36.39	B
ATOM	3371	CB	LEU	B	240	29.435	9.509	29.557	1.00	27.79	B
ATOM	3372	CG	LEU	B	240	29.508	10.513	30.690	1.00	29.69	B
ATOM	3373	CD1	LEU	B	240	30.942	10.583	31.194	1.00	30.85	B



ATOM	3374	CD2	LEU	B	240	29.032	11.874	30.202	1.00	21.59	B
ATOM	3375	C	LEU	B	240	28.168	8.673	27.610	1.00	38.07	B
ATOM	3376	O	LEU	B	240	28.503	9.450	26.722	1.00	34.28	B
ATOM	3377	N	GLY	B	241	27.900	7.388	27.380	1.00	41.68	B
ATOM	3378	CA	GLY	B	241	28.026	6.836	26.041	1.00	43.13	B
ATOM	3379	C	GLY	B	241	29.493	6.588	25.717	1.00	45.49	B
ATOM	3380	O	GLY	B	241	30.274	6.251	26.603	1.00	47.59	B
ATOM	3381	N	ALA	B	242	29.882	6.754	24.457	1.00	44.97	B
ATOM	3382	CA	ALA	B	242	31.272	6.549	24.078	1.00	43.27	B
ATOM	3383	CB	ALA	B	242	31.369	6.048	22.666	1.00	43.85	B
ATOM	3384	C	ALA	B	242	32.029	7.847	24.203	1.00	43.58	B
ATOM	3385	O	ALA	B	242	31.602	8.877	23.694	1.00	46.79	B
ATOM	3386	N	VAL	B	243	33.154	7.791	24.899	1.00	43.90	B
ATOM	3387	CA	VAL	B	243	33.995	8.956	25.088	1.00	45.15	B
ATOM	3388	CB	VAL	B	243	34.213	9.237	26.561	1.00	41.04	B
ATOM	3389	CG1	VAL	B	243	35.072	10.480	26.729	1.00	42.50	B
ATOM	3390	CG2	VAL	B	243	32.882	9.414	27.232	1.00	46.97	B
ATOM	3391	C	VAL	B	243	35.338	8.649	24.442	1.00	49.51	B
ATOM	3392	O	VAL	B	243	35.942	7.606	24.719	1.00	53.18	B
ATOM	3393	N	GLY	B	244	35.797	9.557	23.587	1.00	46.10	B
ATOM	3394	CA	GLY	B	244	37.046	9.343	22.903	1.00	45.94	B
ATOM	3395	C	GLY	B	244	38.098	10.409	23.107	1.00	49.17	B
ATOM	3396	O	GLY	B	244	38.265	10.946	24.209	1.00	49.15	B
ATOM	3397	N	THR	B	245	38.809	10.716	22.024	1.00	51.75	B
ATOM	3398	CA	THR	B	245	39.898	11.685	22.055	1.00	51.61	B
ATOM	3399	CB	THR	B	245	40.769	11.560	20.776	1.00	50.87	B
ATOM	3400	OG1	THR	B	245	39.935	11.583	19.610	1.00	54.40	B
ATOM	3401	CG2	THR	B	245	41.532	10.245	20.795	1.00	43.64	B
ATOM	3402	C	THR	B	245	39.442	13.115	22.264	1.00	51.21	B
ATOM	3403	O	THR	B	245	40.195	13.940	22.781	1.00	53.72	B
ATOM	3404	N	SER	B	246	38.206	13.406	21.871	1.00	52.18	B
ATOM	3405	CA	SER	B	246	37.649	14.743	22.059	1.00	52.11	B
ATOM	3406	CB	SER	B	246	36.619	15.067	20.977	1.00	53.99	B
ATOM	3407	OG	SER	B	246	37.102	14.741	19.688	1.00	64.44	B
ATOM	3408	C	SER	B	246	36.952	14.726	23.414	1.00	49.45	B
ATOM	3409	O	SER	B	246	36.090	13.880	23.659	1.00	48.06	B
ATOM	3410	N	ALA	B	247	37.337	15.651	24.287	1.00	47.65	B
ATOM	3411	CA	ALA	B	247	36.747	15.759	25.614	1.00	47.77	B
ATOM	3412	CB	ALA	B	247	37.324	16.959	26.333	1.00	47.73	B
ATOM	3413	C	ALA	B	247	35.221	15.873	25.569	1.00	48.47	B
ATOM	3414	O	ALA	B	247	34.641	16.428	24.639	1.00	50.29	B
ATOM	3415	N	VAL	B	248	34.575	15.330	26.585	1.00	46.82	B
ATOM	3416	CA	VAL	B	248	33.133	15.383	26.681	1.00	46.36	B
ATOM	3417	CB	VAL	B	248	32.516	13.981	26.698	1.00	46.49	B
ATOM	3418	CG1	VAL	B	248	31.044	14.066	27.053	1.00	44.07	B
ATOM	3419	CG2	VAL	B	248	32.701	13.319	25.349	1.00	46.22	B
ATOM	3420	C	VAL	B	248	32.803	16.074	27.988	1.00	49.23	B
ATOM	3421	O	VAL	B	248	33.256	15.656	29.057	1.00	51.26	B
ATOM	3422	N	SER	B	249	32.018	17.138	27.893	1.00	48.19	B
ATOM	3423	CA	SER	B	249	31.609	17.903	29.060	1.00	46.49	B
ATOM	3424	CB	SER	B	249	31.191	19.308	28.626	1.00	44.33	B
ATOM	3425	OG	SER	B	249	30.934	20.145	29.733	1.00	42.86	B
ATOM	3426	C	SER	B	249	30.430	17.193	29.703	1.00	45.02	B
ATOM	3427	O	SER	B	249	29.502	16.800	29.003	1.00	42.57	B
ATOM	3428	N	LEU	B	250	30.463	17.006	31.022	1.00	45.38	B
ATOM	3429	CA	LEU	B	250	29.336	16.354	31.700	1.00	46.18	B
ATOM	3430	CB	LEU	B	250	29.716	15.920	33.121	1.00	47.35	B
ATOM	3431	CG	LEU	B	250	30.926	14.995	33.318	1.00	50.12	B



ATOM	3432	CD1	LEU	B	250	30.880	14.434	34.742	1.00	42.80	B
ATOM	3433	CD2	LEU	B	250	30.915	13.859	32.294	1.00	47.40	B
ATOM	3434	C	LEU	B	250	28.164	17.340	31.765	1.00	44.55	B
ATOM	3435	O	LEU	B	250	27.020	16.954	32.031	1.00	40.92	B
ATOM	3436	N	GLY	B	251	28.468	18.613	31.512	1.00	38.11	B
ATOM	3437	CA	GLY	B	251	27.451	19.640	31.545	1.00	39.35	B
ATOM	3438	C	GLY	B	251	26.857	19.780	32.930	1.00	38.25	B
ATOM	3439	O	GLY	B	251	25.637	19.768	33.106	1.00	42.31	B
ATOM	3440	N	LEU	B	252	27.733	19.922	33.911	1.00	34.29	B
ATOM	3441	CA	LEU	B	252	27.326	20.043	35.294	1.00	36.24	B
ATOM	3442	CB	LEU	B	252	28.352	19.364	36.206	1.00	32.99	B
ATOM	3443	CG	LEU	B	252	28.547	17.852	36.082	1.00	30.21	B
ATOM	3444	CD1	LEU	B	252	29.689	17.451	36.982	1.00	24.12	B
ATOM	3445	CD2	LEU	B	252	27.276	17.110	36.449	1.00	27.28	B
ATOM	3446	C	LEU	B	252	27.169	21.480	35.757	1.00	39.41	B
ATOM	3447	O	LEU	B	252	27.865	22.375	35.294	1.00	43.64	B
ATOM	3448	N	THR	B	253	26.243	21.688	36.682	1.00	38.02	B
ATOM	3449	CA	THR	B	253	26.016	22.996	37.271	1.00	37.82	B
ATOM	3450	CB	THR	B	253	24.796	23.700	36.677	1.00	40.67	B
ATOM	3451	OG1	THR	B	253	25.162	24.342	35.450	1.00	47.87	B
ATOM	3452	CG2	THR	B	253	24.254	24.724	37.659	1.00	27.23	B
ATOM	3453	C	THR	B	253	25.729	22.771	38.736	1.00	39.11	B
ATOM	3454	O	THR	B	253	24.958	21.868	39.088	1.00	40.91	B
ATOM	3455	N	ALA	B	254	26.361	23.574	39.584	1.00	35.35	B
ATOM	3456	CA	ALA	B	254	26.126	23.492	41.016	1.00	36.35	B
ATOM	3457	CB	ALA	B	254	27.360	23.962	41.786	1.00	29.54	B
ATOM	3458	C	ALA	B	254	24.922	24.406	41.314	1.00	41.67	B
ATOM	3459	O	ALA	B	254	24.836	25.539	40.826	1.00	44.92	B
ATOM	3460	N	ASN	B	255	23.989	23.904	42.108	1.00	40.95	B
ATOM	3461	CA	ASN	B	255	22.796	24.660	42.463	1.00	36.68	B
ATOM	3462	CB	ASN	B	255	21.566	24.036	41.819	1.00	32.94	B
ATOM	3463	CG	ASN	B	255	21.675	23.942	40.341	1.00	30.27	B
ATOM	3464	OD1	ASN	B	255	21.160	24.783	39.626	1.00	37.84	B
ATOM	3465	ND2	ASN	B	255	22.343	22.912	39.862	1.00	40.27	B
ATOM	3466	C	ASN	B	255	22.568	24.596	43.953	1.00	35.83	B
ATOM	3467	O	ASN	B	255	22.895	23.593	44.585	1.00	40.02	B
ATOM	3468	N	TYR	B	256	22.004	25.654	44.521	1.00	34.15	B
ATOM	3469	CA	TYR	B	256	21.655	25.612	45.933	1.00	30.18	B
ATOM	3470	CB	TYR	B	256	21.647	27.002	46.559	1.00	24.06	B
ATOM	3471	CG	TYR	B	256	22.988	27.687	46.675	1.00	26.70	B
ATOM	3472	CD1	TYR	B	256	23.343	28.712	45.795	1.00	26.24	B
ATOM	3473	CE1	TYR	B	256	24.530	29.427	45.955	1.00	32.40	B
ATOM	3474	CD2	TYR	B	256	23.861	27.379	47.715	1.00	24.57	B
ATOM	3475	CE2	TYR	B	256	25.056	28.081	47.887	1.00	30.47	B
ATOM	3476	CZ	TYR	B	256	25.387	29.108	47.007	1.00	35.56	B
ATOM	3477	OH	TYR	B	256	26.559	29.817	47.178	1.00	29.70	B
ATOM	3478	C	TYR	B	256	20.226	25.042	45.980	1.00	29.03	B
ATOM	3479	O	TYR	B	256	19.391	25.350	45.128	1.00	28.10	B
ATOM	3480	N	ALA	B	257	19.959	24.173	46.941	1.00	31.45	B
ATOM	3481	CA	ALA	B	257	18.626	23.614	47.112	1.00	33.79	B
ATOM	3482	CB	ALA	B	257	18.606	22.164	46.739	1.00	36.58	B
ATOM	3483	C	ALA	B	257	18.339	23.781	48.595	1.00	40.06	B
ATOM	3484	O	ALA	B	257	19.263	23.907	49.405	1.00	37.56	B
ATOM	3485	N	ARG	B	258	17.070	23.805	48.960	1.00	46.77	B
ATOM	3486	CA	ARG	B	258	16.736	23.969	50.367	1.00	53.74	B
ATOM	3487	CB	ARG	B	258	15.509	24.870	50.531	1.00	59.02	B
ATOM	3488	CG	ARG	B	258	15.714	26.319	50.133	1.00	59.88	B
ATOM	3489	CD	ARG	B	258	14.404	27.057	50.243	1.00	69.10	B



ATOM	3490	NE	ARG	B	258	13.882	27.004	51.605	1.00	78.61	B
ATOM	3491	CZ	ARG	B	258	12.611	27.224	51.923	1.00	83.09	B
ATOM	3492	NH1	ARG	B	258	11.732	27.506	50.972	1.00	87.22	B
ATOM	3493	NH2	ARG	B	258	12.219	27.169	53.190	1.00	84.52	B
ATOM	3494	C	ARG	B	258	16.468	22.623	51.009	1.00	55.40	B
ATOM	3495	O	ARG	B	258	15.737	21.791	50.457	1.00	55.46	B
ATOM	3496	N	THR	B	259	17.058	22.430	52.183	1.00	56.01	B
ATOM	3497	CA	THR	B	259	16.915	21.194	52.932	1.00	58.80	B
ATOM	3498	CB	THR	B	259	18.159	20.915	53.753	1.00	60.30	B
ATOM	3499	OG1	THR	B	259	18.521	22.094	54.479	1.00	62.86	B
ATOM	3500	CG2	THR	B	259	19.306	20.503	52.853	1.00	65.59	B
ATOM	3501	C	THR	B	259	15.755	21.277	53.887	1.00	62.14	B
ATOM	3502	O	THR	B	259	14.654	20.827	53.576	1.00	61.18	B
ATOM	3503	N	GLY	B	260	16.027	21.863	55.054	1.00	68.48	B
ATOM	3504	CA	GLY	B	260	15.025	22.024	56.094	1.00	69.86	B
ATOM	3505	C	GLY	B	260	13.984	23.075	55.777	1.00	70.03	B
ATOM	3506	O	GLY	B	260	13.201	22.915	54.839	1.00	68.26	B
ATOM	3507	N	GLY	B	261	13.970	24.153	56.554	1.00	74.13	B
ATOM	3508	CA	GLY	B	261	12.991	25.206	56.319	1.00	77.67	B
ATOM	3509	C	GLY	B	261	13.580	26.609	56.274	1.00	78.87	B
ATOM	3510	O	GLY	B	261	13.815	27.164	55.198	1.00	79.92	B
ATOM	3511	N	GLN	B	262	13.821	27.187	57.444	1.00	78.05	B
ATOM	3512	CA	GLN	B	262	14.379	28.525	57.529	1.00	77.99	B
ATOM	3513	CB	GLN	B	262	14.347	29.002	58.978	1.00	86.19	B
ATOM	3514	CG	GLN	B	262	14.416	30.511	59.179	1.00	95.99	B
ATOM	3515	CD	GLN	B	262	13.097	31.198	58.859	1.00	100.91	B
ATOM	3516	OE1	GLN	B	262	12.753	32.222	59.459	1.00	103.29	B
ATOM	3517	NE2	GLN	B	262	12.353	30.642	57.900	1.00	103.10	B
ATOM	3518	C	GLN	B	262	15.821	28.546	57.034	1.00	73.93	B
ATOM	3519	O	GLN	B	262	16.688	27.869	57.592	1.00	74.56	B
ATOM	3520	N	VAL	B	263	16.073	29.318	55.984	1.00	67.20	B
ATOM	3521	CA	VAL	B	263	17.421	29.435	55.456	1.00	61.21	B
ATOM	3522	CB	VAL	B	263	17.400	29.914	53.998	1.00	55.97	B
ATOM	3523	CG1	VAL	B	263	18.815	30.121	53.502	1.00	52.05	B
ATOM	3524	CG2	VAL	B	263	16.661	28.905	53.126	1.00	48.38	B
ATOM	3525	C	VAL	B	263	18.133	30.452	56.336	1.00	60.58	B
ATOM	3526	O	VAL	B	263	17.505	31.348	56.869	1.00	63.79	B
ATOM	3527	N	THR	B	264	19.440	30.330	56.485	1.00	59.49	B
ATOM	3528	CA	THR	B	264	20.157	31.245	57.353	1.00	59.72	B
ATOM	3529	CB	THR	B	264	20.328	30.581	58.696	1.00	57.63	B
ATOM	3530	OG1	THR	B	264	19.035	30.191	59.170	1.00	54.09	B
ATOM	3531	CG2	THR	B	264	21.008	31.500	59.679	1.00	52.49	B
ATOM	3532	C	THR	B	264	21.513	31.664	56.807	1.00	65.90	B
ATOM	3533	O	THR	B	264	22.200	30.880	56.161	1.00	69.63	B
ATOM	3534	N	ALA	B	265	21.903	32.905	57.074	1.00	70.04	B
ATOM	3535	CA	ALA	B	265	23.178	33.427	56.585	1.00	71.83	B
ATOM	3536	CB	ALA	B	265	23.352	34.872	57.019	1.00	73.16	B
ATOM	3537	C	ALA	B	265	24.373	32.610	57.050	1.00	72.52	B
ATOM	3538	O	ALA	B	265	24.316	31.917	58.071	1.00	72.83	B
ATOM	3539	N	GLY	B	266	25.459	32.709	56.289	1.00	73.95	B
ATOM	3540	CA	GLY	B	266	26.676	31.987	56.617	1.00	74.15	B
ATOM	3541	C	GLY	B	266	27.294	31.306	55.411	1.00	72.00	B
ATOM	3542	O	GLY	B	266	26.840	31.486	54.276	1.00	71.05	B
ATOM	3543	N	ASN	B	267	28.331	30.514	55.651	1.00	70.46	B
ATOM	3544	CA	ASN	B	267	28.991	29.805	54.565	1.00	69.21	B
ATOM	3545	CB	ASN	B	267	30.467	29.577	54.895	1.00	75.46	B
ATOM	3546	CG	ASN	B	267	31.303	30.827	54.705	1.00	82.33	B
ATOM	3547	OD1	ASN	B	267	32.526	30.807	54.865	1.00	85.69	B



ATOM	3548	ND2	ASN	B	267	30.647	31.925	54.353	1.00	82.59	B
ATOM	3549	C	ASN	B	267	28.336	28.465	54.227	1.00	64.44	B
ATOM	3550	O	ASN	B	267	27.702	27.825	55.071	1.00	56.70	B
ATOM	3551	N	VAL	B	268	28.490	28.067	52.970	1.00	61.46	B
ATOM	3552	CA	VAL	B	268	27.956	26.812	52.473	1.00	60.68	B
ATOM	3553	CB	VAL	B	268	26.757	27.041	51.537	1.00	60.04	B
ATOM	3554	CG1	VAL	B	268	26.255	25.714	50.999	1.00	59.59	B
ATOM	3555	CG2	VAL	B	268	25.648	27.747	52.283	1.00	61.81	B
ATOM	3556	C	VAL	B	268	29.070	26.129	51.692	1.00	60.85	B
ATOM	3557	O	VAL	B	268	29.458	26.579	50.614	1.00	61.07	B
ATOM	3558	N	GLN	B	269	29.604	25.056	52.256	1.00	60.59	B
ATOM	3559	CA	GLN	B	269	30.673	24.312	51.610	1.00	63.15	B
ATOM	3560	CB	GLN	B	269	31.962	24.442	52.420	1.00	65.20	B
ATOM	3561	CG	GLN	B	269	32.707	25.751	52.213	1.00	71.77	B
ATOM	3562	CD	GLN	B	269	33.842	25.943	53.215	1.00	79.78	B
ATOM	3563	OE1	GLN	B	269	34.648	25.038	53.445	1.00	82.19	B
ATOM	3564	NE2	GLN	B	269	33.912	27.132	53.811	1.00	82.36	B
ATOM	3565	C	GLN	B	269	30.280	22.847	51.460	1.00	64.59	B
ATOM	3566	O	GLN	B	269	29.470	22.326	52.235	1.00	65.27	B
ATOM	3567	N	SER	B	270	30.835	22.182	50.454	1.00	64.78	B
ATOM	3568	CA	SER	B	270	30.504	20.782	50.240	1.00	63.48	B
ATOM	3569	CB	SER	B	270	29.104	20.660	49.647	1.00	63.53	B
ATOM	3570	OG	SER	B	270	28.762	19.296	49.496	1.00	69.22	B
ATOM	3571	C	SER	B	270	31.489	20.001	49.379	1.00	61.80	B
ATOM	3572	O	SER	B	270	32.125	20.540	48.466	1.00	64.03	B
ATOM	3573	N	ILE	B	271	31.601	18.713	49.693	1.00	59.47	B
ATOM	3574	CA	ILE	B	271	32.490	17.788	48.996	1.00	52.99	B
ATOM	3575	CB	ILE	B	271	33.538	17.241	49.961	1.00	56.46	B
ATOM	3576	CG2	ILE	B	271	34.727	18.210	50.031	1.00	58.27	B
ATOM	3577	CG1	ILE	B	271	32.887	17.018	51.333	1.00	55.39	B
ATOM	3578	CD1	ILE	B	271	33.877	16.834	52.480	1.00	58.16	B
ATOM	3579	C	ILE	B	271	31.667	16.650	48.418	1.00	46.51	B
ATOM	3580	O	ILE	B	271	30.938	15.965	49.131	1.00	46.11	B
ATOM	3581	N	ILE	B	272	31.781	16.478	47.108	1.00	41.88	B
ATOM	3582	CA	ILE	B	272	31.045	15.456	46.381	1.00	37.01	B
ATOM	3583	CB	ILE	B	272	30.093	16.101	45.356	1.00	36.10	B
ATOM	3584	CG2	ILE	B	272	29.288	15.039	44.625	1.00	32.58	B
ATOM	3585	CG1	ILE	B	272	29.144	17.053	46.077	1.00	44.11	B
ATOM	3586	CD1	ILE	B	272	28.227	17.828	45.141	1.00	51.23	B
ATOM	3587	C	ILE	B	272	31.976	14.520	45.626	1.00	36.59	B
ATOM	3588	O	ILE	B	272	32.981	14.935	45.049	1.00	35.79	B
ATOM	3589	N	GLY	B	273	31.636	13.246	45.614	1.00	35.00	B
ATOM	3590	CA	GLY	B	273	32.470	12.323	44.892	1.00	36.20	B
ATOM	3591	C	GLY	B	273	31.851	12.043	43.552	1.00	36.68	B
ATOM	3592	O	GLY	B	273	30.631	11.849	43.459	1.00	36.92	B
ATOM	3593	N	VAL	B	274	32.681	12.059	42.510	1.00	34.01	B
ATOM	3594	CA	VAL	B	274	32.205	11.746	41.175	1.00	30.90	B
ATOM	3595	CB	VAL	B	274	32.517	12.857	40.150	1.00	29.36	B
ATOM	3596	CG1	VAL	B	274	31.669	12.638	38.903	1.00	26.39	B
ATOM	3597	CG2	VAL	B	274	32.215	14.227	40.732	1.00	26.01	B
ATOM	3598	C	VAL	B	274	32.952	10.481	40.798	1.00	32.12	B
ATOM	3599	O	VAL	B	274	34.173	10.485	40.694	1.00	32.10	B
ATOM	3600	N	THR	B	275	32.208	9.395	40.619	1.00	34.67	B
ATOM	3601	CA	THR	B	275	32.785	8.102	40.289	1.00	36.64	B
ATOM	3602	CB	THR	B	275	32.257	7.017	41.250	1.00	38.71	B
ATOM	3603	OG1	THR	B	275	32.759	7.279	42.559	1.00	43.63	B
ATOM	3604	CG2	THR	B	275	32.691	5.612	40.806	1.00	43.32	B
ATOM	3605	C	THR	B	275	32.511	7.649	38.866	1.00	35.82	B



ATOM	3606	O	THR	B	275	31.380	7.318	38.519	1.00	36.62	B
ATOM	3607	N	PHE	B	276	33.562	7.619	38.055	1.00	35.05	B
ATOM	3608	CA	PHE	B	276	33.455	7.174	36.676	1.00	31.86	B
ATOM	3609	CB	PHE	B	276	34.567	7.801	35.826	1.00	30.13	B
ATOM	3610	CG	PHE	B	276	34.369	9.254	35.565	1.00	31.90	B
ATOM	3611	CD1	PHE	B	276	34.760	10.202	36.499	1.00	32.35	B
ATOM	3612	CD2	PHE	B	276	33.716	9.678	34.404	1.00	36.57	B
ATOM	3613	CE1	PHE	B	276	34.501	11.566	36.287	1.00	37.33	B
ATOM	3614	CE2	PHE	B	276	33.449	11.036	34.178	1.00	35.47	B
ATOM	3615	CZ	PHE	B	276	33.842	11.982	35.124	1.00	36.46	B
ATOM	3616	C	PHE	B	276	33.555	5.652	36.625	1.00	30.15	B
ATOM	3617	O	PHE	B	276	34.536	5.069	37.083	1.00	27.92	B
ATOM	3618	N	VAL	B	277	32.534	5.015	36.066	1.00	29.51	B
ATOM	3619	CA	VAL	B	277	32.521	3.570	35.975	1.00	29.22	B
ATOM	3620	CB	VAL	B	277	31.138	3.014	36.283	1.00	32.02	B
ATOM	3621	CG1	VAL	B	277	31.212	1.509	36.404	1.00	29.01	B
ATOM	3622	CG2	VAL	B	277	30.613	3.637	37.566	1.00	30.27	B
ATOM	3623	C	VAL	B	277	32.934	3.099	34.603	1.00	28.19	B
ATOM	3624	O	VAL	B	277	32.370	3.522	33.610	1.00	27.93	B
ATOM	3625	N	TYR	B	278	33.926	2.214	34.571	1.00	30.01	B
ATOM	3626	CA	TYR	B	278	34.462	1.663	33.337	1.00	28.31	B
ATOM	3627	CB	TYR	B	278	35.967	1.476	33.452	1.00	25.77	B
ATOM	3628	CG	TYR	B	278	36.704	2.778	33.527	1.00	22.97	B
ATOM	3629	CD1	TYR	B	278	36.689	3.534	34.694	1.00	18.95	B
ATOM	3630	CE1	TYR	B	278	37.353	4.776	34.762	1.00	24.89	B
ATOM	3631	CD2	TYR	B	278	37.396	3.277	32.414	1.00	18.84	B
ATOM	3632	CE2	TYR	B	278	38.058	4.504	32.468	1.00	25.97	B
ATOM	3633	CZ	TYR	B	278	38.036	5.252	33.654	1.00	28.43	B
ATOM	3634	OH	TYR	B	278	38.721	6.450	33.745	1.00	27.64	B
ATOM	3635	C	TYR	B	278	33.855	0.352	32.936	1.00	30.69	B
ATOM	3636	O	TYR	B	278	33.704	-0.550	33.761	1.00	31.74	B
ATOM	3637	N	GLN	B	279	33.516	0.248	31.654	1.00	31.66	B
ATOM	3638	CA	GLN	B	279	32.929	-0.981	31.136	1.00	33.20	B
ATOM	3639	CB	GLN	B	279	32.192	-0.707	29.823	1.00	25.85	B
ATOM	3640	CG	GLN	B	279	31.515	-1.947	29.271	1.00	29.79	B
ATOM	3641	CD	GLN	B	279	30.952	-1.770	27.867	1.00	39.78	B
ATOM	3642	OE1	GLN	B	279	30.094	-2.559	27.445	1.00	42.77	B
ATOM	3643	NE2	GLN	B	279	31.440	-0.756	27.127	1.00	29.64	B
ATOM	3644	C	GLN	B	279	33.999	-2.077	30.932	1.00	33.35	B
ATOM	3645	O	GLN	B	279	33.714	-3.246	31.263	1.00	36.20	B
ATOM	3646	OXT	GLN	B	279	35.109	-1.764	30.445	1.00	28.25	B
ATOM	3647	C	GLY	C	1	82.284	93.643	198.276	1.00	47.80	C
ATOM	3648	O	GLY	C	1	82.098	92.491	197.905	1.00	52.86	C
ATOM	3649	N	GLY	C	1	84.585	94.037	198.871	1.00	52.40	C
ATOM	3650	CA	GLY	C	1	83.542	94.367	197.873	1.00	49.51	C
ATOM	3651	N	VAL	C	2	81.435	94.295	199.063	1.00	42.64	C
ATOM	3652	CA	VAL	C	2	80.189	93.678	199.493	1.00	37.51	C
ATOM	3653	CB	VAL	C	2	79.977	93.837	201.003	1.00	34.81	C
ATOM	3654	CG1	VAL	C	2	78.587	93.368	201.366	1.00	37.50	C
ATOM	3655	CG2	VAL	C	2	81.021	93.025	201.772	1.00	27.99	C
ATOM	3656	C	VAL	C	2	79.038	94.322	198.738	1.00	37.64	C
ATOM	3657	O	VAL	C	2	78.920	95.547	198.713	1.00	37.96	C
ATOM	3658	N	ALA	C	3	78.197	93.500	198.105	1.00	39.34	C
ATOM	3659	CA	ALA	C	3	77.072	94.026	197.327	1.00	35.95	C
ATOM	3660	CB	ALA	C	3	77.373	93.914	195.857	1.00	30.78	C
ATOM	3661	C	ALA	C	3	75.717	93.409	197.609	1.00	33.14	C
ATOM	3662	O	ALA	C	3	75.601	92.220	197.864	1.00	37.44	C
ATOM	3663	N	LEU	C	4	74.689	94.243	197.568	1.00	30.88	C



ATOM	3664	CA	LEU	C	4	73.339	93.782	197.788	1.00	29.83	C
ATOM	3665	CB	LEU	C	4	72.447	94.942	198.210	1.00	27.49	C
ATOM	3666	CG	LEU	C	4	72.827	95.684	199.485	1.00	21.82	C
ATOM	3667	CD1	LEU	C	4	71.697	96.632	199.872	1.00	20.80	C
ATOM	3668	CD2	LEU	C	4	73.091	94.693	200.575	1.00	18.02	C
ATOM	3669	C	LEU	C	4	72.830	93.199	196.474	1.00	31.65	C
ATOM	3670	O	LEU	C	4	73.256	93.636	195.391	1.00	32.97	C
ATOM	3671	N	GLY	C	5	71.920	92.228	196.577	1.00	29.09	C
ATOM	3672	CA	GLY	C	5	71.356	91.580	195.402	1.00	23.89	C
ATOM	3673	C	GLY	C	5	70.178	92.295	194.771	1.00	26.39	C
ATOM	3674	O	GLY	C	5	69.595	91.796	193.829	1.00	34.76	C
ATOM	3675	N	ALA	C	6	69.807	93.457	195.287	1.00	27.47	C
ATOM	3676	CA	ALA	C	6	68.706	94.232	194.715	1.00	28.27	C
ATOM	3677	CB	ALA	C	6	67.398	93.854	195.371	1.00	24.07	C
ATOM	3678	C	ALA	C	6	68.986	95.709	194.949	1.00	28.88	C
ATOM	3679	O	ALA	C	6	69.741	96.064	195.847	1.00	37.35	C
ATOM	3680	N	THR	C	7	68.381	96.574	194.157	1.00	22.34	C
ATOM	3681	CA	THR	C	7	68.588	97.996	194.333	1.00	21.97	C
ATOM	3682	CB	THR	C	7	68.821	98.709	192.985	1.00	22.33	C
ATOM	3683	OG1	THR	C	7	67.610	98.704	192.208	1.00	16.75	C
ATOM	3684	CG2	THR	C	7	69.964	98.022	192.215	1.00	15.39	C
ATOM	3685	C	THR	C	7	67.382	98.605	195.014	1.00	26.64	C
ATOM	3686	O	THR	C	7	67.234	99.826	195.062	1.00	28.57	C
ATOM	3687	N	ARG	C	8	66.510	97.740	195.523	1.00	29.51	C
ATOM	3688	CA	ARG	C	8	65.297	98.161	196.232	1.00	29.70	C
ATOM	3689	CB	ARG	C	8	64.341	98.940	195.329	1.00	22.70	C
ATOM	3690	CG	ARG	C	8	63.508	98.056	194.400	1.00	25.09	C
ATOM	3691	CD	ARG	C	8	63.740	98.379	192.936	1.00	24.16	C
ATOM	3692	NE	ARG	C	8	63.441	99.779	192.632	1.00	23.82	C
ATOM	3693	CZ	ARG	C	8	64.368	100.712	192.443	1.00	19.89	C
ATOM	3694	NH1	ARG	C	8	64.009	101.953	192.177	1.00	20.93	C
ATOM	3695	NH2	ARG	C	8	65.651	100.392	192.505	1.00	12.20	C
ATOM	3696	C	ARG	C	8	64.574	96.922	196.752	1.00	30.90	C
ATOM	3697	O	ARG	C	8	64.866	95.795	196.361	1.00	31.96	C
ATOM	3698	N	VAL	C	9	63.621	97.143	197.637	1.00	31.14	C
ATOM	3699	CA	VAL	C	9	62.881	96.059	198.222	1.00	27.86	C
ATOM	3700	CB	VAL	C	9	63.436	95.721	199.588	1.00	23.41	C
ATOM	3701	CG1	VAL	C	9	62.515	94.790	200.300	1.00	31.32	C
ATOM	3702	CG2	VAL	C	9	64.789	95.086	199.433	1.00	25.66	C
ATOM	3703	C	VAL	C	9	61.430	96.469	198.364	1.00	31.99	C
ATOM	3704	O	VAL	C	9	61.113	97.600	198.750	1.00	29.12	C
ATOM	3705	N	ILE	C	10	60.551	95.541	198.006	1.00	34.65	C
ATOM	3706	CA	ILE	C	10	59.131	95.764	198.121	1.00	32.90	C
ATOM	3707	CB	ILE	C	10	58.405	95.355	196.862	1.00	25.94	C
ATOM	3708	CG2	ILE	C	10	56.918	95.553	197.035	1.00	23.95	C
ATOM	3709	CG1	ILE	C	10	58.895	96.215	195.709	1.00	26.72	C
ATOM	3710	CD1	ILE	C	10	58.573	97.686	195.857	1.00	23.90	C
ATOM	3711	C	ILE	C	10	58.665	94.897	199.262	1.00	36.81	C
ATOM	3712	O	ILE	C	10	58.809	93.676	199.220	1.00	34.85	C
ATOM	3713	N	TYR	C	11	58.143	95.537	200.300	1.00	38.74	C
ATOM	3714	CA	TYR	C	11	57.644	94.800	201.451	1.00	39.72	C
ATOM	3715	CB	TYR	C	11	58.020	95.488	202.755	1.00	35.97	C
ATOM	3716	CG	TYR	C	11	58.011	94.548	203.926	1.00	40.02	C
ATOM	3717	CD1	TYR	C	11	59.179	93.906	204.327	1.00	42.31	C
ATOM	3718	CE1	TYR	C	11	59.184	92.994	205.382	1.00	41.14	C
ATOM	3719	CD2	TYR	C	11	56.833	94.259	204.612	1.00	35.73	C
ATOM	3720	CE2	TYR	C	11	56.827	93.343	205.669	1.00	37.89	C
ATOM	3721	CZ	TYR	C	11	58.012	92.713	206.045	1.00	39.50	C



ATOM	3722	OH	TYR	C	11	58.037	91.789	207.065	1.00	38.93	C
ATOM	3723	C	TYR	C	11	56.130	94.737	201.353	1.00	39.73	C
ATOM	3724	O	TYR	C	11	55.454	95.749	201.560	1.00	32.07	C
ATOM	3725	N	PRO	C	12	55.581	93.546	201.024	1.00	42.99	C
ATOM	3726	CD	PRO	C	12	56.323	92.335	200.634	1.00	42.10	C
ATOM	3727	CA	PRO	C	12	54.135	93.319	200.890	1.00	42.62	C
ATOM	3728	CB	PRO	C	12	54.051	91.920	200.271	1.00	41.25	C
ATOM	3729	CG	PRO	C	12	55.403	91.728	199.619	1.00	41.11	C
ATOM	3730	C	PRO	C	12	53.489	93.355	202.258	1.00	39.78	C
ATOM	3731	O	PRO	C	12	53.844	92.558	203.123	1.00	37.52	C
ATOM	3732	N	ALA	C	13	52.559	94.279	202.465	1.00	42.06	C
ATOM	3733	CA	ALA	C	13	51.891	94.360	203.756	1.00	47.94	C
ATOM	3734	CB	ALA	C	13	50.793	95.409	203.719	1.00	47.72	C
ATOM	3735	C	ALA	C	13	51.310	92.983	204.095	1.00	52.32	C
ATOM	3736	O	ALA	C	13	50.589	92.377	203.292	1.00	52.58	C
ATOM	3737	N	GLY	C	14	51.645	92.484	205.279	1.00	55.11	C
ATOM	3738	CA	GLY	C	14	51.150	91.188	205.691	1.00	55.68	C
ATOM	3739	C	GLY	C	14	52.262	90.167	205.801	1.00	58.97	C
ATOM	3740	O	GLY	C	14	52.311	89.412	206.774	1.00	60.10	C
ATOM	3741	N	GLN	C	15	53.152	90.137	204.809	1.00	59.01	C
ATOM	3742	CA	GLN	C	15	54.267	89.194	204.806	1.00	58.86	C
ATOM	3743	CB	GLN	C	15	55.280	89.563	203.722	1.00	60.40	C
ATOM	3744	CG	GLN	C	15	54.695	89.693	202.329	1.00	68.08	C
ATOM	3745	CD	GLN	C	15	54.804	88.425	201.503	1.00	72.86	C
ATOM	3746	OE1	GLN	C	15	54.378	87.353	201.929	1.00	76.38	C
ATOM	3747	NE2	GLN	C	15	55.372	88.546	200.304	1.00	75.46	C
ATOM	3748	C	GLN	C	15	54.952	89.223	206.163	1.00	60.53	C
ATOM	3749	O	GLN	C	15	55.174	90.285	206.741	1.00	61.41	C
ATOM	3750	N	LYS	C	16	55.280	88.053	206.682	1.00	63.48	C
ATOM	3751	CA	LYS	C	16	55.945	87.996	207.968	1.00	66.28	C
ATOM	3752	CB	LYS	C	16	55.995	86.560	208.473	1.00	72.55	C
ATOM	3753	CG	LYS	C	16	56.490	86.423	209.906	1.00	81.73	C
ATOM	3754	CD	LYS	C	16	56.700	84.956	210.296	1.00	89.61	C
ATOM	3755	CE	LYS	C	16	55.530	84.061	209.847	1.00	92.46	C
ATOM	3756	NZ	LYS	C	16	54.196	84.530	210.332	1.00	92.32	C
ATOM	3757	C	LYS	C	16	57.364	88.524	207.808	1.00	66.00	C
ATOM	3758	O	LYS	C	16	57.938	89.067	208.747	1.00	69.14	C
ATOM	3759	N	GLN	C	17	57.922	88.374	206.609	1.00	62.74	C
ATOM	3760	CA	GLN	C	17	59.287	88.819	206.349	1.00	59.20	C
ATOM	3761	CB	GLN	C	17	60.260	87.982	207.173	1.00	58.18	C
ATOM	3762	CG	GLN	C	17	60.110	86.513	206.890	1.00	62.51	C
ATOM	3763	CD	GLN	C	17	61.372	85.733	207.151	1.00	65.45	C
ATOM	3764	OE1	GLN	C	17	61.894	85.727	208.274	1.00	62.42	C
ATOM	3765	NE2	GLN	C	17	61.878	85.060	206.109	1.00	62.28	C
ATOM	3766	C	GLN	C	17	59.704	88.728	204.878	1.00	53.91	C
ATOM	3767	O	GLN	C	17	59.260	87.852	204.145	1.00	53.08	C
ATOM	3768	N	VAL	C	18	60.569	89.643	204.460	1.00	48.87	C
ATOM	3769	CA	VAL	C	18	61.064	89.648	203.099	1.00	45.24	C
ATOM	3770	CB	VAL	C	18	60.771	90.964	202.399	1.00	44.20	C
ATOM	3771	CG1	VAL	C	18	61.381	90.956	201.016	1.00	45.77	C
ATOM	3772	CG2	VAL	C	18	59.276	91.170	202.307	1.00	48.76	C
ATOM	3773	C	VAL	C	18	62.562	89.468	203.211	1.00	47.01	C
ATOM	3774	O	VAL	C	18	63.167	89.863	204.206	1.00	49.52	C
ATOM	3775	N	GLN	C	19	63.175	88.871	202.203	1.00	44.25	C
ATOM	3776	CA	GLN	C	19	64.597	88.658	202.287	1.00	43.81	C
ATOM	3777	CB	GLN	C	19	64.881	87.169	202.383	1.00	47.35	C
ATOM	3778	CG	GLN	C	19	64.106	86.340	201.401	1.00	58.37	C
ATOM	3779	CD	GLN	C	19	64.022	84.901	201.837	1.00	60.14	C



ATOM	3780	OE1	GLN	C	19	63.414	84.597	202.863	1.00	63.64	C
ATOM	3781	NE2	GLN	C	19	64.640	84.005	201.069	1.00	66.29	C
ATOM	3782	C	GLN	C	19	65.369	89.292	201.156	1.00	40.82	C
ATOM	3783	O	GLN	C	19	64.862	89.439	200.059	1.00	39.81	C
ATOM	3784	N	LEU	C	20	66.601	89.685	201.471	1.00	37.67	C
ATOM	3785	CA	LEU	C	20	67.517	90.334	200.548	1.00	32.34	C
ATOM	3786	CB	LEU	C	20	67.717	91.790	200.983	1.00	27.58	C
ATOM	3787	CG	LEU	C	20	68.627	92.722	200.172	1.00	27.41	C
ATOM	3788	CD1	LEU	C	20	68.004	93.002	198.819	1.00	23.64	C
ATOM	3789	CD2	LEU	C	20	68.838	94.024	200.934	1.00	26.17	C
ATOM	3790	C	LEU	C	20	68.855	89.577	200.572	1.00	32.15	C
ATOM	3791	O	LEU	C	20	69.261	89.047	201.601	1.00	28.32	C
ATOM	3792	N	ALA	C	21	69.535	89.531	199.434	1.00	34.28	C
ATOM	3793	CA	ALA	C	21	70.799	88.820	199.346	1.00	32.51	C
ATOM	3794	CB	ALA	C	21	70.892	88.071	198.017	1.00	26.24	C
ATOM	3795	C	ALA	C	21	71.969	89.757	199.469	1.00	33.56	C
ATOM	3796	O	ALA	C	21	71.919	90.901	199.022	1.00	30.14	C
ATOM	3797	N	VAL	C	22	73.031	89.243	200.072	1.00	35.99	C
ATOM	3798	CA	VAL	C	22	74.253	89.998	200.239	1.00	39.04	C
ATOM	3799	CB	VAL	C	22	74.565	90.356	201.691	1.00	37.76	C
ATOM	3800	CG1	VAL	C	22	75.364	91.650	201.728	1.00	33.72	C
ATOM	3801	CG2	VAL	C	22	73.304	90.429	202.494	1.00	38.39	C
ATOM	3802	C	VAL	C	22	75.334	89.048	199.829	1.00	43.75	C
ATOM	3803	O	VAL	C	22	75.321	87.869	200.201	1.00	47.48	C
ATOM	3804	N	THR	C	23	76.288	89.569	199.086	1.00	44.44	C
ATOM	3805	CA	THR	C	23	77.380	88.760	198.635	1.00	45.58	C
ATOM	3806	CB	THR	C	23	77.140	88.340	197.189	1.00	47.38	C
ATOM	3807	OG1	THR	C	23	78.369	87.889	196.616	1.00	58.41	C
ATOM	3808	CG2	THR	C	23	76.591	89.501	196.388	1.00	50.60	C
ATOM	3809	C	THR	C	23	78.661	89.568	198.782	1.00	44.89	C
ATOM	3810	O	THR	C	23	78.683	90.765	198.507	1.00	41.14	C
ATOM	3811	N	ASN	C	24	79.709	88.892	199.249	1.00	47.08	C
ATOM	3812	CA	ASN	C	24	81.024	89.473	199.470	1.00	44.67	C
ATOM	3813	CB	ASN	C	24	81.499	89.123	200.882	1.00	41.68	C
ATOM	3814	CG	ASN	C	24	82.942	89.541	201.142	1.00	46.70	C
ATOM	3815	OD1	ASN	C	24	83.464	90.445	200.490	1.00	42.01	C
ATOM	3816	ND2	ASN	C	24	83.585	88.894	202.113	1.00	41.52	C
ATOM	3817	C	ASN	C	24	82.000	88.926	198.435	1.00	47.88	C
ATOM	3818	O	ASN	C	24	82.336	87.741	198.451	1.00	46.41	C
ATOM	3819	N	ASN	C	25	82.446	89.807	197.542	1.00	52.95	C
ATOM	3820	CA	ASN	C	25	83.385	89.477	196.460	1.00	56.72	C
ATOM	3821	CB	ASN	C	25	83.471	90.632	195.461	1.00	53.45	C
ATOM	3822	CG	ASN	C	25	82.174	90.883	194.750	1.00	52.94	C
ATOM	3823	OD1	ASN	C	25	81.096	90.660	195.300	1.00	54.34	C
ATOM	3824	ND2	ASN	C	25	82.265	91.372	193.521	1.00	56.79	C
ATOM	3825	C	ASN	C	25	84.802	89.194	196.933	1.00	58.94	C
ATOM	3826	O	ASN	C	25	85.382	88.155	196.624	1.00	62.02	C
ATOM	3827	N	ASP	C	26	85.360	90.149	197.661	1.00	59.08	C
ATOM	3828	CA	ASP	C	26	86.714	90.046	198.159	1.00	61.73	C
ATOM	3829	CB	ASP	C	26	86.929	91.072	199.250	1.00	65.93	C
ATOM	3830	CG	ASP	C	26	86.784	92.482	198.741	1.00	67.09	C
ATOM	3831	OD1	ASP	C	26	86.874	93.410	199.573	1.00	70.36	C
ATOM	3832	OD2	ASP	C	26	86.581	92.658	197.513	1.00	65.25	C
ATOM	3833	C	ASP	C	26	87.110	88.679	198.654	1.00	63.97	C
ATOM	3834	O	ASP	C	26	86.846	88.308	199.793	1.00	65.66	C
ATOM	3835	N	GLU	C	27	87.771	87.942	197.775	1.00	67.29	C
ATOM	3836	CA	GLU	C	27	88.231	86.599	198.067	1.00	70.86	C
ATOM	3837	CB	GLU	C	27	89.165	86.126	196.945	1.00	77.52	C



ATOM	3838	CG	GLU	C	27	88.407	85.691	195.682	1.00	91.83	C
ATOM	3839	CD	GLU	C	27	89.160	85.953	194.379	1.00	98.28	C
ATOM	3840	OE1	GLU	C	27	90.337	85.536	194.265	1.00	102.35	C
ATOM	3841	OE2	GLU	C	27	88.558	86.568	193.465	1.00	100.04	C
ATOM	3842	C	GLU	C	27	88.915	86.478	199.414	1.00	69.08	C
ATOM	3843	O	GLU	C	27	88.969	85.395	199.977	1.00	69.88	C
ATOM	3844	N	ASN	C	28	89.423	87.579	199.951	1.00	69.03	C
ATOM	3845	CA	ASN	C	28	90.096	87.488	201.236	1.00	73.05	C
ATOM	3846	CB	ASN	C	28	91.540	87.001	201.032	1.00	79.79	C
ATOM	3847	CG	ASN	C	28	92.294	87.807	199.977	1.00	84.46	C
ATOM	3848	OD1	ASN	C	28	93.371	87.406	199.526	1.00	80.13	C
ATOM	3849	ND2	ASN	C	28	91.729	88.950	199.583	1.00	86.62	C
ATOM	3850	C	ASN	C	28	90.076	88.771	202.043	1.00	71.95	C
ATOM	3851	O	ASN	C	28	90.868	89.680	201.822	1.00	75.63	C
ATOM	3852	N	SER	C	29	89.159	88.812	202.997	1.00	70.78	C
ATOM	3853	CA	SER	C	29	88.962	89.951	203.885	1.00	69.08	C
ATOM	3854	CB	SER	C	29	88.990	91.270	203.100	1.00	69.88	C
ATOM	3855	OG	SER	C	29	87.969	91.304	202.118	1.00	62.99	C
ATOM	3856	C	SER	C	29	87.588	89.751	204.516	1.00	65.21	C
ATOM	3857	O	SER	C	29	86.578	89.731	203.821	1.00	66.37	C
ATOM	3858	N	THR	C	30	87.549	89.582	205.828	1.00	61.05	C
ATOM	3859	CA	THR	C	30	86.281	89.371	206.496	1.00	58.61	C
ATOM	3860	CB	THR	C	30	86.486	88.713	207.866	1.00	57.95	C
ATOM	3861	OG1	THR	C	30	87.288	87.536	207.713	1.00	61.24	C
ATOM	3862	CG2	THR	C	30	85.163	88.297	208.449	1.00	63.15	C
ATOM	3863	C	THR	C	30	85.561	90.695	206.672	1.00	55.48	C
ATOM	3864	O	THR	C	30	86.173	91.759	206.592	1.00	57.77	C
ATOM	3865	N	TYR	C	31	84.253	90.625	206.885	1.00	51.80	C
ATOM	3866	CA	TYR	C	31	83.438	91.816	207.090	1.00	50.13	C
ATOM	3867	CB	TYR	C	31	82.756	92.238	205.796	1.00	50.26	C
ATOM	3868	CG	TYR	C	31	83.644	92.926	204.802	1.00	52.64	C
ATOM	3869	CD1	TYR	C	31	83.973	92.318	203.595	1.00	52.05	C
ATOM	3870	CE1	TYR	C	31	84.730	92.985	202.646	1.00	56.63	C
ATOM	3871	CD2	TYR	C	31	84.104	94.219	205.037	1.00	55.05	C
ATOM	3872	CE2	TYR	C	31	84.859	94.895	204.094	1.00	56.52	C
ATOM	3873	CZ	TYR	C	31	85.165	94.275	202.903	1.00	59.00	C
ATOM	3874	OH	TYR	C	31	85.881	94.963	201.957	1.00	67.61	C
ATOM	3875	C	TYR	C	31	82.346	91.581	208.124	1.00	49.09	C
ATOM	3876	O	TYR	C	31	81.870	90.458	208.318	1.00	51.62	C
ATOM	3877	N	LEU	C	32	81.957	92.650	208.798	1.00	44.10	C
ATOM	3878	CA	LEU	C	32	80.883	92.569	209.762	1.00	41.27	C
ATOM	3879	CB	LEU	C	32	81.241	93.294	211.052	1.00	47.86	C
ATOM	3880	CG	LEU	C	32	81.985	92.484	212.111	1.00	50.85	C
ATOM	3881	CD1	LEU	C	32	82.422	93.419	213.240	1.00	52.23	C
ATOM	3882	CD2	LEU	C	32	81.085	91.364	212.621	1.00	46.14	C
ATOM	3883	C	LEU	C	32	79.733	93.276	209.078	1.00	41.23	C
ATOM	3884	O	LEU	C	32	79.837	94.447	208.689	1.00	36.29	C
ATOM	3885	N	ILE	C	33	78.644	92.548	208.896	1.00	38.59	C
ATOM	3886	CA	ILE	C	33	77.491	93.113	208.255	1.00	35.09	C
ATOM	3887	CB	ILE	C	33	76.791	92.060	207.392	1.00	37.49	C
ATOM	3888	CG2	ILE	C	33	75.614	92.689	206.630	1.00	35.15	C
ATOM	3889	CG1	ILE	C	33	77.819	91.425	206.447	1.00	38.22	C
ATOM	3890	CD1	ILE	C	33	78.638	92.426	205.654	1.00	27.16	C
ATOM	3891	C	ILE	C	33	76.565	93.600	209.340	1.00	35.31	C
ATOM	3892	O	ILE	C	33	76.190	92.847	210.243	1.00	34.27	C
ATOM	3893	N	GLN	C	34	76.216	94.874	209.249	1.00	33.45	C
ATOM	3894	CA	GLN	C	34	75.324	95.500	210.207	1.00	34.45	C
ATOM	3895	CB	GLN	C	34	76.099	96.529	211.019	1.00	38.51	C



ATOM	3896	CG	GLN	C	34	75.587	96.769	212.409	1.00	38.42	C
ATOM	3897	CD	GLN	C	34	76.488	97.705	213.177	1.00	42.59	C
ATOM	3898	OE1	GLN	C	34	76.633	98.874	212.825	1.00	49.60	C
ATOM	3899	NE2	GLN	C	34	77.115	97.193	214.226	1.00	44.72	C
ATOM	3900	C	GLN	C	34	74.249	96.181	209.373	1.00	32.15	C
ATOM	3901	O	GLN	C	34	74.546	97.088	208.605	1.00	31.59	C
ATOM	3902	N	SER	C	35	73.003	95.748	209.526	1.00	30.76	C
ATOM	3903	CA	SER	C	35	71.911	96.317	208.746	1.00	32.03	C
ATOM	3904	CB	SER	C	35	71.287	95.218	207.892	1.00	33.64	C
ATOM	3905	OG	SER	C	35	72.294	94.434	207.296	1.00	41.25	C
ATOM	3906	C	SER	C	35	70.815	96.974	209.573	1.00	29.68	C
ATOM	3907	O	SER	C	35	70.572	96.590	210.706	1.00	36.57	C
ATOM	3908	N	TRP	C	36	70.145	97.958	208.999	1.00	24.09	C
ATOM	3909	CA	TRP	C	36	69.044	98.622	209.689	1.00	27.31	C
ATOM	3910	CB	TRP	C	36	69.550	99.611	210.738	1.00	18.33	C
ATOM	3911	CG	TRP	C	36	70.132	100.862	210.182	1.00	19.19	C
ATOM	3912	CD2	TRP	C	36	71.478	101.051	209.738	1.00	20.58	C
ATOM	3913	CE2	TRP	C	36	71.582	102.380	209.261	1.00	24.78	C
ATOM	3914	CE3	TRP	C	36	72.610	100.226	209.699	1.00	17.43	C
ATOM	3915	CD1	TRP	C	36	69.488	102.042	209.966	1.00	24.90	C
ATOM	3916	NE1	TRP	C	36	70.352	102.965	209.411	1.00	26.58	C
ATOM	3917	CZ2	TRP	C	36	72.777	102.905	208.748	1.00	18.18	C
ATOM	3918	CZ3	TRP	C	36	73.805	100.749	209.191	1.00	19.76	C
ATOM	3919	CH2	TRP	C	36	73.875	102.076	208.724	1.00	18.14	C
ATOM	3920	C	TRP	C	36	68.160	99.348	208.683	1.00	27.98	C
ATOM	3921	O	TRP	C	36	68.480	99.450	207.502	1.00	27.18	C
ATOM	3922	N	VAL	C	37	67.035	99.847	209.163	1.00	26.68	C
ATOM	3923	CA	VAL	C	37	66.117	100.536	208.294	1.00	27.00	C
ATOM	3924	CB	VAL	C	37	64.882	99.671	208.016	1.00	24.02	C
ATOM	3925	CG1	VAL	C	37	63.925	100.408	207.113	1.00	27.07	C
ATOM	3926	CG2	VAL	C	37	65.310	98.374	207.385	1.00	25.57	C
ATOM	3927	C	VAL	C	37	65.683	101.830	208.932	1.00	27.29	C
ATOM	3928	O	VAL	C	37	65.201	101.838	210.055	1.00	33.48	C
ATOM	3929	N	GLU	C	38	65.874	102.925	208.213	1.00	25.74	C
ATOM	3930	CA	GLU	C	38	65.474	104.230	208.699	1.00	27.08	C
ATOM	3931	CB	GLU	C	38	66.529	105.265	208.336	1.00	24.24	C
ATOM	3932	CG	GLU	C	38	67.872	104.944	208.949	1.00	30.81	C
ATOM	3933	CD	GLU	C	38	68.965	105.798	208.390	1.00	32.52	C
ATOM	3934	OE1	GLU	C	38	68.605	106.849	207.810	1.00	27.54	C
ATOM	3935	OE2	GLU	C	38	70.164	105.428	208.538	1.00	30.88	C
ATOM	3936	C	GLU	C	38	64.173	104.538	207.996	1.00	27.46	C
ATOM	3937	O	GLU	C	38	63.880	103.940	206.963	1.00	29.90	C
ATOM	3938	N	ASN	C	39	63.375	105.433	208.563	1.00	27.37	C
ATOM	3939	CA	ASN	C	39	62.126	105.789	207.924	1.00	28.73	C
ATOM	3940	CB	ASN	C	39	61.070	106.202	208.943	1.00	30.19	C
ATOM	3941	CG	ASN	C	39	61.435	107.470	209.695	1.00	41.20	C
ATOM	3942	OD1	ASN	C	39	62.264	108.272	209.247	1.00	41.54	C
ATOM	3943	ND2	ASN	C	39	60.794	107.671	210.841	1.00	41.71	C
ATOM	3944	C	ASN	C	39	62.408	106.935	206.961	1.00	32.17	C
ATOM	3945	O	ASN	C	39	63.562	107.356	206.799	1.00	28.30	C
ATOM	3946	N	ALA	C	40	61.348	107.439	206.332	1.00	34.05	C
ATOM	3947	CA	ALA	C	40	61.470	108.502	205.353	1.00	34.87	C
ATOM	3948	CB	ALA	C	40	60.108	108.941	204.906	1.00	39.82	C
ATOM	3949	C	ALA	C	40	62.250	109.683	205.861	1.00	37.43	C
ATOM	3950	O	ALA	C	40	63.016	110.278	205.123	1.00	41.98	C
ATOM	3951	N	ASP	C	41	62.068	110.034	207.122	1.00	39.93	C
ATOM	3952	CA	ASP	C	41	62.791	111.172	207.655	1.00	43.39	C
ATOM	3953	CB	ASP	C	41	62.053	111.746	208.851	1.00	47.27	C



ATOM	3954	CG	ASP	C	41	60.762	112.410	208.455	1.00	52.51	C
ATOM	3955	OD1	ASP	C	41	60.797	113.241	207.521	1.00	57.76	C
ATOM	3956	OD2	ASP	C	41	59.720	112.105	209.073	1.00	50.84	C
ATOM	3957	C	ASP	C	41	64.236	110.878	208.027	1.00	44.53	C
ATOM	3958	O	ASP	C	41	64.946	111.756	208.498	1.00	48.94	C
ATOM	3959	N	GLY	C	42	64.681	109.649	207.810	1.00	40.84	C
ATOM	3960	CA	GLY	C	42	66.052	109.322	208.130	1.00	34.57	C
ATOM	3961	C	GLY	C	42	66.255	108.859	209.552	1.00	36.10	C
ATOM	3962	O	GLY	C	42	67.383	108.572	209.939	1.00	34.98	C
ATOM	3963	N	VAL	C	43	65.188	108.771	210.344	1.00	37.80	C
ATOM	3964	CA	VAL	C	43	65.374	108.330	211.719	1.00	38.56	C
ATOM	3965	CB	VAL	C	43	64.458	109.106	212.709	1.00	31.38	C
ATOM	3966	CG1	VAL	C	43	63.760	110.228	212.003	1.00	29.16	C
ATOM	3967	CG2	VAL	C	43	63.483	108.176	213.377	1.00	38.44	C
ATOM	3968	C	VAL	C	43	65.190	106.824	211.898	1.00	42.60	C
ATOM	3969	O	VAL	C	43	64.305	106.207	211.287	1.00	45.76	C
ATOM	3970	N	LYS	C	44	66.040	106.242	212.742	1.00	39.87	C
ATOM	3971	CA	LYS	C	44	65.985	104.822	213.003	1.00	40.62	C
ATOM	3972	CB	LYS	C	44	67.302	104.330	213.619	1.00	41.67	C
ATOM	3973	CG	LYS	C	44	68.552	104.505	212.777	1.00	43.65	C
ATOM	3974	CD	LYS	C	44	69.558	105.391	213.481	1.00	49.04	C
ATOM	3975	CE	LYS	C	44	70.829	105.539	212.673	1.00	50.04	C
ATOM	3976	NZ	LYS	C	44	71.483	104.222	212.479	1.00	56.49	C
ATOM	3977	C	LYS	C	44	64.856	104.472	213.960	1.00	41.70	C
ATOM	3978	O	LYS	C	44	65.089	104.319	215.159	1.00	42.96	C
ATOM	3979	N	ASP	C	45	63.627	104.386	213.469	1.00	41.66	C
ATOM	3980	CA	ASP	C	45	62.562	103.957	214.365	1.00	41.32	C
ATOM	3981	CB	ASP	C	45	61.199	104.457	213.927	1.00	43.12	C
ATOM	3982	CG	ASP	C	45	60.987	104.342	212.440	1.00	44.28	C
ATOM	3983	OD1	ASP	C	45	61.558	103.415	211.825	1.00	42.26	C
ATOM	3984	OD2	ASP	C	45	60.234	105.175	211.899	1.00	35.65	C
ATOM	3985	C	ASP	C	45	62.647	102.457	214.210	1.00	45.07	C
ATOM	3986	O	ASP	C	45	63.520	101.955	213.490	1.00	50.93	C
ATOM	3987	N	GLY	C	46	61.757	101.719	214.843	1.00	44.81	C
ATOM	3988	CA	GLY	C	46	61.882	100.279	214.721	1.00	44.13	C
ATOM	3989	C	GLY	C	46	60.863	99.666	213.809	1.00	44.90	C
ATOM	3990	O	GLY	C	46	60.587	98.472	213.911	1.00	44.16	C
ATOM	3991	N	ARG	C	47	60.302	100.477	212.917	1.00	44.00	C
ATOM	3992	CA	ARG	C	47	59.293	99.983	212.002	1.00	42.69	C
ATOM	3993	CB	ARG	C	47	58.968	101.035	210.958	1.00	50.35	C
ATOM	3994	CG	ARG	C	47	57.617	101.670	211.182	1.00	61.04	C
ATOM	3995	CD	ARG	C	47	57.598	102.519	212.430	1.00	68.87	C
ATOM	3996	NE	ARG	C	47	56.246	102.988	212.711	1.00	82.07	C
ATOM	3997	CZ	ARG	C	47	55.298	102.235	213.265	1.00	90.71	C
ATOM	3998	NH1	ARG	C	47	55.562	100.980	213.604	1.00	95.97	C
ATOM	3999	NH2	ARG	C	47	54.082	102.729	213.476	1.00	94.06	C
ATOM	4000	C	ARG	C	47	59.700	98.685	211.329	1.00	42.80	C
ATOM	4001	O	ARG	C	47	58.876	97.800	211.122	1.00	42.21	C
ATOM	4002	N	PHE	C	48	60.976	98.559	210.993	1.00	40.39	C
ATOM	4003	CA	PHE	C	48	61.445	97.339	210.353	1.00	39.64	C
ATOM	4004	CB	PHE	C	48	61.660	97.552	208.839	1.00	38.30	C
ATOM	4005	CG	PHE	C	48	60.389	97.752	208.084	1.00	32.16	C
ATOM	4006	CD1	PHE	C	48	59.823	99.017	207.973	1.00	29.81	C
ATOM	4007	CD2	PHE	C	48	59.691	96.656	207.590	1.00	31.79	C
ATOM	4008	CE1	PHE	C	48	58.583	99.189	207.398	1.00	26.97	C
ATOM	4009	CE2	PHE	C	48	58.447	96.812	207.011	1.00	26.86	C
ATOM	4010	CZ	PHE	C	48	57.886	98.075	206.915	1.00	29.66	C
ATOM	4011	C	PHE	C	48	62.723	96.869	211.003	1.00	36.34	C



ATOM	4012	O	PHE	C	48	63.535	97.681	211.397	1.00	34.61	C
ATOM	4013	N	ILE	C	49	62.892	95.554	211.106	1.00	35.46	C
ATOM	4014	CA	ILE	C	49	64.080	94.996	211.716	1.00	37.43	C
ATOM	4015	CB	ILE	C	49	63.723	94.375	213.072	1.00	41.64	C
ATOM	4016	CG2	ILE	C	49	64.938	93.703	213.700	1.00	36.12	C
ATOM	4017	CG1	ILE	C	49	63.239	95.492	213.999	1.00	42.64	C
ATOM	4018	CD1	ILE	C	49	62.438	94.997	215.178	1.00	50.85	C
ATOM	4019	C	ILE	C	49	64.713	93.979	210.789	1.00	36.63	C
ATOM	4020	O	ILE	C	49	64.030	93.183	210.163	1.00	40.23	C
ATOM	4021	N	VAL	C	50	66.032	94.015	210.705	1.00	32.70	C
ATOM	4022	CA	VAL	C	50	66.751	93.123	209.820	1.00	33.80	C
ATOM	4023	CB	VAL	C	50	67.737	93.927	208.927	1.00	37.22	C
ATOM	4024	CG1	VAL	C	50	68.394	93.013	207.898	1.00	36.52	C
ATOM	4025	CG2	VAL	C	50	67.001	95.074	208.253	1.00	37.37	C
ATOM	4026	C	VAL	C	50	67.543	92.125	210.623	1.00	32.90	C
ATOM	4027	O	VAL	C	50	68.100	92.472	211.660	1.00	35.67	C
ATOM	4028	N	THR	C	51	67.601	90.886	210.153	1.00	29.99	C
ATOM	4029	CA	THR	C	51	68.378	89.864	210.845	1.00	30.68	C
ATOM	4030	CB	THR	C	51	67.495	88.848	211.603	1.00	35.47	C
ATOM	4031	OG1	THR	C	51	66.548	88.268	210.696	1.00	40.09	C
ATOM	4032	CG2	THR	C	51	66.753	89.512	212.744	1.00	40.38	C
ATOM	4033	C	THR	C	51	69.180	89.079	209.831	1.00	32.09	C
ATOM	4034	O	THR	C	51	68.758	88.886	208.693	1.00	34.34	C
ATOM	4035	N	PRO	C	52	70.375	88.650	210.220	1.00	31.87	C
ATOM	4036	CD	PRO	C	52	71.052	87.490	209.626	1.00	31.15	C
ATOM	4037	CA	PRO	C	52	70.900	88.934	211.557	1.00	32.99	C
ATOM	4038	CB	PRO	C	52	72.058	87.947	211.704	1.00	30.92	C
ATOM	4039	CG	PRO	C	52	72.382	87.552	210.299	1.00	35.51	C
ATOM	4040	C	PRO	C	52	71.362	90.377	211.642	1.00	35.74	C
ATOM	4041	O	PRO	C	52	71.961	90.904	210.710	1.00	39.69	C
ATOM	4042	N	PRO	C	53	71.085	91.043	212.764	1.00	33.93	C
ATOM	4043	CD	PRO	C	53	70.457	90.552	214.002	1.00	32.30	C
ATOM	4044	CA	PRO	C	53	71.505	92.435	212.898	1.00	32.39	C
ATOM	4045	CB	PRO	C	53	70.969	92.820	214.273	1.00	32.88	C
ATOM	4046	CG	PRO	C	53	70.994	91.499	215.023	1.00	29.64	C
ATOM	4047	C	PRO	C	53	73.012	92.638	212.784	1.00	32.10	C
ATOM	4048	O	PRO	C	53	73.462	93.742	212.516	1.00	31.38	C
ATOM	4049	N	LEU	C	54	73.787	91.576	212.985	1.00	34.31	C
ATOM	4050	CA	LEU	C	54	75.247	91.667	212.920	1.00	35.90	C
ATOM	4051	CB	LEU	C	54	75.799	92.224	214.226	1.00	36.76	C
ATOM	4052	CG	LEU	C	54	77.317	92.330	214.328	1.00	38.09	C
ATOM	4053	CD1	LEU	C	54	77.794	93.603	213.622	1.00	43.96	C
ATOM	4054	CD2	LEU	C	54	77.714	92.359	215.778	1.00	37.68	C
ATOM	4055	C	LEU	C	54	75.872	90.307	212.705	1.00	38.16	C
ATOM	4056	O	LEU	C	54	75.654	89.404	213.513	1.00	43.88	C
ATOM	4057	N	PHE	C	55	76.663	90.157	211.646	1.00	36.15	C
ATOM	4058	CA	PHE	C	55	77.302	88.872	211.359	1.00	35.98	C
ATOM	4059	CB	PHE	C	55	76.318	87.917	210.702	1.00	32.13	C
ATOM	4060	CG	PHE	C	55	75.825	88.388	209.374	1.00	39.81	C
ATOM	4061	CD1	PHE	C	55	76.430	87.959	208.198	1.00	41.92	C
ATOM	4062	CD2	PHE	C	55	74.770	89.294	209.294	1.00	42.59	C
ATOM	4063	CE1	PHE	C	55	75.993	88.425	206.951	1.00	42.45	C
ATOM	4064	CE2	PHE	C	55	74.325	89.767	208.056	1.00	47.62	C
ATOM	4065	CZ	PHE	C	55	74.938	89.332	206.880	1.00	44.74	C
ATOM	4066	C	PHE	C	55	78.496	89.032	210.451	1.00	39.55	C
ATOM	4067	O	PHE	C	55	78.666	90.067	209.805	1.00	42.02	C
ATOM	4068	N	ALA	C	56	79.316	87.990	210.385	1.00	42.81	C
ATOM	4069	CA	ALA	C	56	80.517	88.030	209.558	1.00	41.76	C



ATOM	4070	CB	ALA	C	56	81.694	87.514	210.356	1.00	38.75	C
ATOM	4071	C	ALA	C	56	80.428	87.287	208.223	1.00	40.09	C
ATOM	4072	O	ALA	C	56	79.750	86.264	208.084	1.00	37.71	C
ATOM	4073	N	MET	C	57	81.111	87.836	207.232	1.00	39.98	C
ATOM	4074	CA	MET	C	57	81.167	87.232	205.916	1.00	42.59	C
ATOM	4075	CB	MET	C	57	80.494	88.121	204.875	1.00	39.70	C
ATOM	4076	CG	MET	C	57	79.028	88.363	205.128	1.00	43.59	C
ATOM	4077	SD	MET	C	57	78.096	88.358	203.578	1.00	47.27	C
ATOM	4078	CE	MET	C	57	78.721	89.808	202.864	1.00	57.39	C
ATOM	4079	C	MET	C	57	82.656	87.114	205.632	1.00	44.97	C
ATOM	4080	O	MET	C	57	83.342	88.116	205.401	1.00	42.67	C
ATOM	4081	N	LYS	C	58	83.154	85.886	205.679	1.00	47.91	C
ATOM	4082	CA	LYS	C	58	84.564	85.642	205.450	1.00	56.07	C
ATOM	4083	CB	LYS	C	58	85.055	84.555	206.403	1.00	61.66	C
ATOM	4084	CG	LYS	C	58	86.563	84.497	206.557	1.00	66.16	C
ATOM	4085	CD	LYS	C	58	86.969	83.349	207.466	1.00	71.39	C
ATOM	4086	CE	LYS	C	58	88.326	83.603	208.115	1.00	76.59	C
ATOM	4087	NZ	LYS	C	58	88.273	84.763	209.061	1.00	75.59	C
ATOM	4088	C	LYS	C	58	84.839	85.232	204.006	1.00	57.70	C
ATOM	4089	O	LYS	C	58	84.336	84.214	203.535	1.00	60.74	C
ATOM	4090	N	GLY	C	59	85.641	86.031	203.310	1.00	57.50	C
ATOM	4091	CA	GLY	C	59	85.970	85.724	201.931	1.00	57.28	C
ATOM	4092	C	GLY	C	59	84.733	85.666	201.066	1.00	55.51	C
ATOM	4093	O	GLY	C	59	83.659	86.049	201.519	1.00	52.74	C
ATOM	4094	N	LYS	C	60	84.879	85.193	199.829	1.00	56.19	C
ATOM	4095	CA	LYS	C	60	83.748	85.107	198.914	1.00	58.74	C
ATOM	4096	CB	LYS	C	60	84.178	84.546	197.556	1.00	58.13	C
ATOM	4097	CG	LYS	C	60	85.264	85.368	196.874	1.00	61.25	C
ATOM	4098	CD	LYS	C	60	85.233	85.230	195.361	1.00	64.10	C
ATOM	4099	CE	LYS	C	60	83.992	85.892	194.783	1.00	73.21	C
ATOM	4100	NZ	LYS	C	60	83.977	85.900	193.287	1.00	80.41	C
ATOM	4101	C	LYS	C	60	82.681	84.221	199.529	1.00	58.59	C
ATOM	4102	O	LYS	C	60	82.849	83.012	199.624	1.00	61.67	C
ATOM	4103	N	LYS	C	61	81.591	84.843	199.959	1.00	55.11	C
ATOM	4104	CA	LYS	C	61	80.489	84.141	200.595	1.00	50.13	C
ATOM	4105	CB	LYS	C	61	80.600	84.257	202.117	1.00	50.07	C
ATOM	4106	CG	LYS	C	61	80.714	82.926	202.838	1.00	57.49	C
ATOM	4107	CD	LYS	C	61	79.718	82.838	203.992	1.00	60.10	C
ATOM	4108	CE	LYS	C	61	79.980	83.906	205.062	1.00	68.66	C
ATOM	4109	NZ	LYS	C	61	78.938	83.936	206.152	1.00	66.44	C
ATOM	4110	C	LYS	C	61	79.189	84.777	200.136	1.00	47.80	C
ATOM	4111	O	LYS	C	61	79.190	85.806	199.462	1.00	46.03	C
ATOM	4112	N	GLU	C	62	78.076	84.158	200.497	1.00	47.17	C
ATOM	4113	CA	GLU	C	62	76.771	84.684	200.130	1.00	47.93	C
ATOM	4114	CB	GLU	C	62	76.308	84.048	198.824	1.00	48.27	C
ATOM	4115	CG	GLU	C	62	75.526	84.990	197.939	1.00	65.47	C
ATOM	4116	CD	GLU	C	62	74.027	84.739	197.986	1.00	72.46	C
ATOM	4117	OE1	GLU	C	62	73.458	84.696	199.101	1.00	77.88	C
ATOM	4118	OE2	GLU	C	62	73.420	84.592	196.899	1.00	72.13	C
ATOM	4119	C	GLU	C	62	75.831	84.336	201.279	1.00	45.06	C
ATOM	4120	O	GLU	C	62	75.842	83.210	201.776	1.00	50.21	C
ATOM	4121	N	ASN	C	63	75.054	85.304	201.742	1.00	39.37	C
ATOM	4122	CA	ASN	C	63	74.136	85.033	202.838	1.00	38.76	C
ATOM	4123	CB	ASN	C	63	74.684	85.489	204.189	1.00	40.89	C
ATOM	4124	CG	ASN	C	63	75.927	84.762	204.587	1.00	45.78	C
ATOM	4125	OD1	ASN	C	63	77.027	85.171	204.237	1.00	50.88	C
ATOM	4126	ND2	ASN	C	63	75.765	83.665	205.313	1.00	47.22	C
ATOM	4127	C	ASN	C	63	72.874	85.778	202.587	1.00	37.28	C



ATOM	4128	O	ASN	C	63	72.804	86.594	201.661	1.00	39.40	C
ATOM	4129	N	THR	C	64	71.885	85.525	203.435	1.00	33.11	C
ATOM	4130	CA	THR	C	64	70.604	86.177	203.283	1.00	34.48	C
ATOM	4131	CB	THR	C	64	69.497	85.156	203.035	1.00	32.27	C
ATOM	4132	OG1	THR	C	64	69.873	84.305	201.948	1.00	44.70	C
ATOM	4133	CG2	THR	C	64	68.197	85.864	202.693	1.00	30.86	C
ATOM	4134	C	THR	C	64	70.163	87.048	204.442	1.00	36.22	C
ATOM	4135	O	THR	C	64	70.185	86.632	205.599	1.00	40.90	C
ATOM	4136	N	LEU	C	65	69.754	88.264	204.112	1.00	36.10	C
ATOM	4137	CA	LEU	C	65	69.246	89.195	205.099	1.00	37.30	C
ATOM	4138	CB	LEU	C	65	69.646	90.622	204.738	1.00	32.48	C
ATOM	4139	CG	LEU	C	65	71.131	90.923	204.855	1.00	30.07	C
ATOM	4140	CD1	LEU	C	65	71.394	92.374	204.544	1.00	31.04	C
ATOM	4141	CD2	LEU	C	65	71.592	90.607	206.250	1.00	36.01	C
ATOM	4142	C	LEU	C	65	67.728	89.063	205.050	1.00	39.45	C
ATOM	4143	O	LEU	C	65	67.158	88.944	203.968	1.00	35.94	C
ATOM	4144	N	ARG	C	66	67.083	89.065	206.215	1.00	41.50	C
ATOM	4145	CA	ARG	C	66	65.629	88.952	206.289	1.00	42.71	C
ATOM	4146	CB	ARG	C	66	65.232	87.708	207.083	1.00	42.21	C
ATOM	4147	CG	ARG	C	66	65.753	86.413	206.491	1.00	50.83	C
ATOM	4148	CD	ARG	C	66	65.505	85.223	207.415	1.00	58.84	C
ATOM	4149	NE	ARG	C	66	66.419	84.115	207.135	1.00	59.81	C
ATOM	4150	CZ	ARG	C	66	66.389	83.383	206.031	1.00	59.51	C
ATOM	4151	NH1	ARG	C	66	65.483	83.636	205.098	1.00	61.29	C
ATOM	4152	NH2	ARG	C	66	67.272	82.406	205.854	1.00	65.54	C
ATOM	4153	C	ARG	C	66	65.074	90.195	206.965	1.00	43.68	C
ATOM	4154	O	ARG	C	66	65.483	90.533	208.080	1.00	47.33	C
ATOM	4155	N	ILE	C	67	64.163	90.880	206.279	1.00	40.46	C
ATOM	4156	CA	ILE	C	67	63.554	92.096	206.805	1.00	39.13	C
ATOM	4157	CB	ILE	C	67	63.305	93.139	205.702	1.00	37.41	C
ATOM	4158	CG2	ILE	C	67	62.526	94.304	206.266	1.00	40.71	C
ATOM	4159	CG1	ILE	C	67	64.627	93.647	205.128	1.00	39.69	C
ATOM	4160	CD1	ILE	C	67	65.271	92.703	204.149	1.00	42.41	C
ATOM	4161	C	ILE	C	67	62.218	91.796	207.476	1.00	42.16	C
ATOM	4162	O	ILE	C	67	61.262	91.321	206.843	1.00	41.63	C
ATOM	4163	N	LEU	C	68	62.143	92.103	208.762	1.00	39.83	C
ATOM	4164	CA	LEU	C	68	60.935	91.845	209.513	1.00	39.35	C
ATOM	4165	CB	LEU	C	68	61.281	91.200	210.846	1.00	38.99	C
ATOM	4166	CG	LEU	C	68	62.266	90.051	210.825	1.00	33.23	C
ATOM	4167	CD1	LEU	C	68	62.496	89.618	212.246	1.00	32.97	C
ATOM	4168	CD2	LEU	C	68	61.728	88.914	209.990	1.00	38.69	C
ATOM	4169	C	LEU	C	68	60.104	93.085	209.780	1.00	42.26	C
ATOM	4170	O	LEU	C	68	60.622	94.144	210.161	1.00	40.16	C
ATOM	4171	N	ASP	C	69	58.799	92.912	209.600	1.00	44.01	C
ATOM	4172	CA	ASP	C	69	57.809	93.949	209.809	1.00	43.20	C
ATOM	4173	CB	ASP	C	69	56.539	93.537	209.082	1.00	41.80	C
ATOM	4174	CG	ASP	C	69	55.394	94.499	209.298	1.00	47.86	C
ATOM	4175	OD1	ASP	C	69	54.324	94.275	208.682	1.00	53.00	C
ATOM	4176	OD2	ASP	C	69	55.551	95.465	210.074	1.00	37.17	C
ATOM	4177	C	ASP	C	69	57.546	94.113	211.302	1.00	47.45	C
ATOM	4178	O	ASP	C	69	56.994	93.231	211.941	1.00	50.90	C
ATOM	4179	N	ALA	C	70	57.959	95.232	211.872	1.00	52.18	C
ATOM	4180	CA	ALA	C	70	57.719	95.460	213.288	1.00	61.22	C
ATOM	4181	CB	ALA	C	70	58.917	96.121	213.930	1.00	61.48	C
ATOM	4182	C	ALA	C	70	56.508	96.365	213.403	1.00	69.44	C
ATOM	4183	O	ALA	C	70	55.789	96.345	214.401	1.00	72.24	C
ATOM	4184	N	THR	C	71	56.291	97.163	212.361	1.00	78.15	C
ATOM	4185	CA	THR	C	71	55.172	98.094	212.324	1.00	84.88	C



ATOM	4186	CB	THR	C	71	55.250	99.043	211.090	1.00	82.25	C
ATOM	4187	OG1	THR	C	71	54.069	99.849	211.037	1.00	83.66	C
ATOM	4188	CG2	THR	C	71	55.378	98.260	209.796	1.00	82.08	C
ATOM	4189	C	THR	C	71	53.848	97.347	212.303	1.00	91.28	C
ATOM	4190	O	THR	C	71	53.427	96.826	211.262	1.00	93.29	C
ATOM	4191	N	ASN	C	72	53.203	97.290	213.466	1.00	95.44	C
ATOM	4192	CA	ASN	C	72	51.920	96.610	213.600	1.00	99.89	C
ATOM	4193	CB	ASN	C	72	51.500	96.567	215.076	1.00	105.66	C
ATOM	4194	CG	ASN	C	72	52.211	95.472	215.860	1.00	110.37	C
ATOM	4195	OD1	ASN	C	72	51.986	95.309	217.063	1.00	110.22	C
ATOM	4196	ND2	ASN	C	72	53.070	94.710	215.179	1.00	112.45	C
ATOM	4197	C	ASN	C	72	50.833	97.299	212.771	1.00	100.19	C
ATOM	4198	O	ASN	C	72	49.906	97.900	213.320	1.00	101.88	C
ATOM	4199	N	ASN	C	73	50.953	97.211	211.449	1.00	98.55	C
ATOM	4200	CA	ASN	C	73	49.984	97.824	210.545	1.00	95.87	C
ATOM	4201	CB	ASN	C	73	48.715	96.965	210.472	1.00	98.58	C
ATOM	4202	CG	ASN	C	73	49.013	95.477	210.405	1.00	101.36	C
ATOM	4203	OD1	ASN	C	73	49.550	94.891	211.351	1.00	101.49	C
ATOM	4204	ND2	ASN	C	73	48.662	94.856	209.286	1.00	100.77	C
ATOM	4205	C	ASN	C	73	49.616	99.234	211.024	1.00	92.07	C
ATOM	4206	O	ASN	C	73	48.463	99.652	210.920	1.00	91.51	C
ATOM	4207	N	GLN	C	74	50.598	99.956	211.560	1.00	86.79	C
ATOM	4208	CA	GLN	C	74	50.375	101.312	212.057	1.00	81.00	C
ATOM	4209	CB	GLN	C	74	51.242	101.557	213.301	1.00	86.33	C
ATOM	4210	CG	GLN	C	74	50.917	100.604	214.467	1.00	92.89	C
ATOM	4211	CD	GLN	C	74	51.999	100.545	215.552	1.00	94.78	C
ATOM	4212	OE1	GLN	C	74	51.852	99.830	216.549	1.00	91.99	C
ATOM	4213	NE2	GLN	C	74	53.087	101.288	215.356	1.00	94.14	C
ATOM	4214	C	GLN	C	74	50.700	102.335	210.973	1.00	74.13	C
ATOM	4215	O	GLN	C	74	50.798	103.534	211.241	1.00	72.76	C
ATOM	4216	N	LEU	C	75	50.859	101.846	209.746	1.00	66.10	C
ATOM	4217	CA	LEU	C	75	51.174	102.696	208.601	1.00	60.39	C
ATOM	4218	CB	LEU	C	75	52.283	102.062	207.752	1.00	49.63	C
ATOM	4219	CG	LEU	C	75	53.652	101.815	208.376	1.00	46.54	C
ATOM	4220	CD1	LEU	C	75	54.421	100.847	207.509	1.00	42.39	C
ATOM	4221	CD2	LEU	C	75	54.403	103.119	208.541	1.00	36.34	C
ATOM	4222	C	LEU	C	75	49.956	102.896	207.709	1.00	60.12	C
ATOM	4223	O	LEU	C	75	49.005	102.118	207.748	1.00	62.73	C
ATOM	4224	N	PRO	C	76	49.971	103.950	206.887	1.00	58.03	C
ATOM	4225	CD	PRO	C	76	50.983	105.014	206.807	1.00	58.07	C
ATOM	4226	CA	PRO	C	76	48.856	104.224	205.981	1.00	59.78	C
ATOM	4227	CB	PRO	C	76	49.387	105.381	205.143	1.00	55.14	C
ATOM	4228	CG	PRO	C	76	50.222	106.117	206.112	1.00	53.65	C
ATOM	4229	C	PRO	C	76	48.579	102.974	205.134	1.00	62.32	C
ATOM	4230	O	PRO	C	76	49.515	102.318	204.681	1.00	62.07	C
ATOM	4231	N	GLN	C	77	47.304	102.650	204.916	1.00	64.58	C
ATOM	4232	CA	GLN	C	77	46.952	101.464	204.137	1.00	64.79	C
ATOM	4233	CB	GLN	C	77	45.908	100.647	204.891	1.00	64.74	C
ATOM	4234	CG	GLN	C	77	46.429	100.094	206.195	1.00	69.48	C
ATOM	4235	CD	GLN	C	77	47.682	99.273	206.002	1.00	72.27	C
ATOM	4236	OE1	GLN	C	77	48.673	99.450	206.716	1.00	72.62	C
ATOM	4237	NE2	GLN	C	77	47.647	98.361	205.033	1.00	72.12	C
ATOM	4238	C	GLN	C	77	46.474	101.720	202.708	1.00	63.22	C
ATOM	4239	O	GLN	C	77	46.150	100.783	201.986	1.00	62.43	C
ATOM	4240	N	ASP	C	78	46.453	102.982	202.298	1.00	61.10	C
ATOM	4241	CA	ASP	C	78	46.018	103.333	200.954	1.00	59.37	C
ATOM	4242	CB	ASP	C	78	45.128	104.577	201.003	1.00	59.11	C
ATOM	4243	CG	ASP	C	78	45.806	105.758	201.668	1.00	63.32	C



ATOM	4244	OD1	ASP	C	78	45.328	106.895	201.486	1.00	65.38	C
ATOM	4245	OD2	ASP	C	78	46.810	105.560	202.379	1.00	68.55	C
ATOM	4246	C	ASP	C	78	47.184	103.589	199.999	1.00	60.48	C
ATOM	4247	O	ASP	C	78	47.009	103.621	198.781	1.00	62.28	C
ATOM	4248	N	ARG	C	79	48.380	103.753	200.548	1.00	60.17	C
ATOM	4249	CA	ARG	C	79	49.550	104.050	199.734	1.00	55.26	C
ATOM	4250	CB	ARG	C	79	49.759	105.558	199.708	1.00	55.07	C
ATOM	4251	CG	ARG	C	79	50.082	106.127	201.084	1.00	55.71	C
ATOM	4252	CD	ARG	C	79	49.861	107.613	201.134	1.00	53.84	C
ATOM	4253	NE	ARG	C	79	48.436	107.893	201.074	1.00	59.74	C
ATOM	4254	CZ	ARG	C	79	47.911	109.095	200.873	1.00	61.98	C
ATOM	4255	NH1	ARG	C	79	48.695	110.155	200.708	1.00	60.35	C
ATOM	4256	NH2	ARG	C	79	46.594	109.227	200.825	1.00	61.13	C
ATOM	4257	C	ARG	C	79	50.780	103.393	200.316	1.00	50.34	C
ATOM	4258	O	ARG	C	79	50.743	102.891	201.437	1.00	50.72	C
ATOM	4259	N	GLU	C	80	51.870	103.405	199.557	1.00	45.81	C
ATOM	4260	CA	GLU	C	80	53.119	102.825	200.032	1.00	41.60	C
ATOM	4261	CB	GLU	C	80	54.104	102.601	198.894	1.00	39.77	C
ATOM	4262	CG	GLU	C	80	53.633	101.772	197.733	1.00	37.34	C
ATOM	4263	CD	GLU	C	80	54.725	101.628	196.689	1.00	36.26	C
ATOM	4264	OE1	GLU	C	80	55.218	100.501	196.481	1.00	29.36	C
ATOM	4265	OE2	GLU	C	80	55.103	102.655	196.084	1.00	39.98	C
ATOM	4266	C	GLU	C	80	53.755	103.836	200.972	1.00	42.77	C
ATOM	4267	O	GLU	C	80	53.494	105.037	200.879	1.00	43.27	C
ATOM	4268	N	SER	C	81	54.587	103.350	201.883	1.00	41.36	C
ATOM	4269	CA	SER	C	81	55.287	104.232	202.794	1.00	38.69	C
ATOM	4270	CB	SER	C	81	54.998	103.849	204.243	1.00	38.68	C
ATOM	4271	OG	SER	C	81	53.618	103.999	204.537	1.00	46.54	C
ATOM	4272	C	SER	C	81	56.760	104.051	202.461	1.00	39.37	C
ATOM	4273	O	SER	C	81	57.229	102.922	202.291	1.00	42.30	C
ATOM	4274	N	LEU	C	82	57.484	105.160	202.336	1.00	37.81	C
ATOM	4275	CA	LEU	C	82	58.907	105.107	202.005	1.00	37.17	C
ATOM	4276	CB	LEU	C	82	59.327	106.400	201.309	1.00	35.02	C
ATOM	4277	CG	LEU	C	82	60.825	106.670	201.142	1.00	37.28	C
ATOM	4278	CD1	LEU	C	82	61.555	105.491	200.547	1.00	27.82	C
ATOM	4279	CD2	LEU	C	82	60.980	107.880	200.265	1.00	38.03	C
ATOM	4280	C	LEU	C	82	59.819	104.858	203.198	1.00	36.51	C
ATOM	4281	O	LEU	C	82	59.673	105.494	204.247	1.00	34.52	C
ATOM	4282	N	PHE	C	83	60.753	103.923	203.022	1.00	34.91	C
ATOM	4283	CA	PHE	C	83	61.733	103.583	204.053	1.00	34.14	C
ATOM	4284	CB	PHE	C	83	61.344	102.308	204.788	1.00	32.45	C
ATOM	4285	CG	PHE	C	83	60.221	102.491	205.751	1.00	39.47	C
ATOM	4286	CD1	PHE	C	83	58.901	102.540	205.310	1.00	32.49	C
ATOM	4287	CD2	PHE	C	83	60.484	102.652	207.110	1.00	42.10	C
ATOM	4288	CE1	PHE	C	83	57.869	102.743	206.204	1.00	30.45	C
ATOM	4289	CE2	PHE	C	83	59.453	102.856	208.012	1.00	35.16	C
ATOM	4290	CZ	PHE	C	83	58.145	102.901	207.552	1.00	40.47	C
ATOM	4291	C	PHE	C	83	63.096	103.382	203.411	1.00	34.89	C
ATOM	4292	O	PHE	C	83	63.203	103.246	202.196	1.00	36.04	C
ATOM	4293	N	TRP	C	84	64.141	103.367	204.229	1.00	32.15	C
ATOM	4294	CA	TRP	C	84	65.468	103.170	203.702	1.00	26.37	C
ATOM	4295	CB	TRP	C	84	66.264	104.457	203.781	1.00	17.45	C
ATOM	4296	CG	TRP	C	84	65.695	105.511	202.912	1.00	21.91	C
ATOM	4297	CD2	TRP	C	84	66.001	105.753	201.528	1.00	16.44	C
ATOM	4298	CE2	TRP	C	84	65.224	106.854	201.116	1.00	16.68	C
ATOM	4299	CE3	TRP	C	84	66.849	105.140	200.597	1.00	22.59	C
ATOM	4300	CD1	TRP	C	84	64.770	106.443	203.266	1.00	21.21	C
ATOM	4301	NE1	TRP	C	84	64.486	107.261	202.196	1.00	23.42	C



ATOM	4302	CZ2	TRP	C	84	65.269	107.360	199.813	1.00	18.40	C
ATOM	4303	CZ3	TRP	C	84	66.895	105.646	199.296	1.00	12.77	C
ATOM	4304	CH2	TRP	C	84	66.111	106.742	198.922	1.00	17.00	C
ATOM	4305	C	TRP	C	84	66.209	102.051	204.385	1.00	29.58	C
ATOM	4306	O	TRP	C	84	66.373	102.045	205.601	1.00	33.29	C
ATOM	4307	N	MET	C	85	66.651	101.107	203.561	1.00	30.91	C
ATOM	4308	CA	MET	C	85	67.382	99.917	203.962	1.00	27.89	C
ATOM	4309	CB	MET	C	85	66.965	98.776	203.028	1.00	27.01	C
ATOM	4310	CG	MET	C	85	67.759	97.494	203.151	1.00	33.69	C
ATOM	4311	SD	MET	C	85	67.324	96.526	204.573	1.00	40.67	C
ATOM	4312	CE	MET	C	85	68.475	95.159	204.440	1.00	31.35	C
ATOM	4313	C	MET	C	85	68.887	100.202	203.863	1.00	28.56	C
ATOM	4314	O	MET	C	85	69.380	100.659	202.820	1.00	27.79	C
ATOM	4315	N	ASN	C	86	69.608	99.942	204.954	1.00	27.95	C
ATOM	4316	CA	ASN	C	86	71.054	100.183	205.010	1.00	25.57	C
ATOM	4317	CB	ASN	C	86	71.393	101.320	206.001	1.00	19.17	C
ATOM	4318	CG	ASN	C	86	70.826	102.676	205.571	1.00	26.85	C
ATOM	4319	OD1	ASN	C	86	69.643	102.963	205.778	1.00	29.10	C
ATOM	4320	ND2	ASN	C	86	71.668	103.512	204.971	1.00	21.29	C
ATOM	4321	C	ASN	C	86	71.816	98.932	205.410	1.00	24.24	C
ATOM	4322	O	ASN	C	86	71.456	98.272	206.367	1.00	28.42	C
ATOM	4323	N	VAL	C	87	72.870	98.613	204.661	1.00	26.20	C
ATOM	4324	CA	VAL	C	87	73.709	97.447	204.923	1.00	21.04	C
ATOM	4325	CB	VAL	C	87	73.517	96.362	203.840	1.00	20.01	C
ATOM	4326	CG1	VAL	C	87	74.441	95.169	204.094	1.00	11.59	C
ATOM	4327	CG2	VAL	C	87	72.053	95.910	203.820	1.00	10.62	C
ATOM	4328	C	VAL	C	87	75.139	97.968	204.897	1.00	27.14	C
ATOM	4329	O	VAL	C	87	75.655	98.412	203.862	1.00	26.21	C
ATOM	4330	N	LYS	C	88	75.745	97.932	206.075	1.00	29.25	C
ATOM	4331	CA	LYS	C	88	77.094	98.406	206.312	1.00	30.45	C
ATOM	4332	CB	LYS	C	88	77.112	99.136	207.645	1.00	26.10	C
ATOM	4333	CG	LYS	C	88	78.440	99.610	208.120	1.00	27.13	C
ATOM	4334	CD	LYS	C	88	78.204	100.714	209.123	1.00	30.18	C
ATOM	4335	CE	LYS	C	88	79.384	100.916	210.032	1.00	34.56	C
ATOM	4336	NZ	LYS	C	88	78.971	101.839	211.098	1.00	33.72	C
ATOM	4337	C	LYS	C	88	78.094	97.272	206.332	1.00	31.26	C
ATOM	4338	O	LYS	C	88	77.827	96.224	206.904	1.00	35.75	C
ATOM	4339	N	ALA	C	89	79.244	97.480	205.701	1.00	32.14	C
ATOM	4340	CA	ALA	C	89	80.280	96.462	205.681	1.00	35.00	C
ATOM	4341	CB	ALA	C	89	80.755	96.228	204.267	1.00	38.93	C
ATOM	4342	C	ALA	C	89	81.436	96.934	206.553	1.00	36.63	C
ATOM	4343	O	ALA	C	89	82.222	97.786	206.157	1.00	38.46	C
ATOM	4344	N	ILE	C	90	81.532	96.374	207.748	1.00	38.33	C
ATOM	4345	CA	ILE	C	90	82.583	96.747	208.680	1.00	44.39	C
ATOM	4346	CB	ILE	C	90	82.106	96.567	210.139	1.00	43.19	C
ATOM	4347	CG2	ILE	C	90	83.239	96.878	211.090	1.00	38.20	C
ATOM	4348	CG1	ILE	C	90	80.894	97.463	210.408	1.00	43.19	C
ATOM	4349	CD1	ILE	C	90	80.269	97.266	211.767	1.00	38.45	C
ATOM	4350	C	ILE	C	90	83.861	95.928	208.494	1.00	50.06	C
ATOM	4351	O	ILE	C	90	83.863	94.692	208.626	1.00	51.70	C
ATOM	4352	N	PRO	C	91	84.972	96.601	208.181	1.00	51.91	C
ATOM	4353	CD	PRO	C	91	85.174	98.016	207.845	1.00	50.07	C
ATOM	4354	CA	PRO	C	91	86.207	95.842	208.008	1.00	54.21	C
ATOM	4355	CB	PRO	C	91	87.122	96.841	207.320	1.00	48.24	C
ATOM	4356	CG	PRO	C	91	86.682	98.124	207.894	1.00	51.18	C
ATOM	4357	C	PRO	C	91	86.719	95.393	209.372	1.00	58.98	C
ATOM	4358	O	PRO	C	91	85.942	95.177	210.294	1.00	58.55	C
ATOM	4359	N	SER	C	92	88.029	95.249	209.497	1.00	66.08	C



ATOM	4360	CA	SER	C	92	88.634	94.815	210.745	1.00	67.26	C
ATOM	4361	CB	SER	C	92	88.958	93.325	210.648	1.00	66.19	C
ATOM	4362	OG	SER	C	92	89.323	92.991	209.315	1.00	67.25	C
ATOM	4363	C	SER	C	92	89.890	95.636	210.954	1.00	70.18	C
ATOM	4364	O	SER	C	92	90.514	96.044	209.985	1.00	72.54	C
ATOM	4365	N	MET	C	93	90.260	95.881	212.207	1.00	75.94	C
ATOM	4366	CA	MET	C	93	91.450	96.679	212.515	1.00	81.70	C
ATOM	4367	CB	MET	C	93	91.393	97.175	213.970	1.00	88.65	C
ATOM	4368	CG	MET	C	93	92.345	98.340	214.300	1.00	98.39	C
ATOM	4369	SD	MET	C	93	94.051	97.929	214.834	1.00	105.77	C
ATOM	4370	CE	MET	C	93	94.070	98.632	216.490	1.00	100.27	C
ATOM	4371	C	MET	C	93	92.754	95.916	212.292	1.00	82.57	C
ATOM	4372	O	MET	C	93	92.954	94.842	212.863	1.00	80.96	C
ATOM	4373	N	ASP	C	94	93.629	96.471	211.451	1.00	84.66	C
ATOM	4374	CA	ASP	C	94	94.923	95.850	211.184	1.00	86.49	C
ATOM	4375	CB	ASP	C	94	95.664	96.511	210.009	1.00	87.53	C
ATOM	4376	CG	ASP	C	94	94.902	96.440	208.697	1.00	92.41	C
ATOM	4377	OD1	ASP	C	94	95.563	96.385	207.631	1.00	87.30	C
ATOM	4378	OD2	ASP	C	94	93.652	96.459	208.726	1.00	94.22	C
ATOM	4379	C	ASP	C	94	95.768	96.062	212.422	1.00	87.82	C
ATOM	4380	O	ASP	C	94	95.988	97.200	212.834	1.00	88.63	C
ATOM	4381	N	LYS	C	95	96.230	94.978	213.030	1.00	88.84	C
ATOM	4382	CA	LYS	C	95	97.086	95.105	214.197	1.00	88.45	C
ATOM	4383	CB	LYS	C	95	97.128	93.790	214.972	1.00	87.51	C
ATOM	4384	CG	LYS	C	95	95.839	93.461	215.706	1.00	85.60	C
ATOM	4385	CD	LYS	C	95	94.725	93.020	214.781	1.00	88.20	C
ATOM	4386	CE	LYS	C	95	94.966	91.618	214.234	1.00	88.04	C
ATOM	4387	NZ	LYS	C	95	93.794	91.111	213.462	1.00	85.88	C
ATOM	4388	C	LYS	C	95	98.457	95.434	213.620	1.00	89.08	C
ATOM	4389	O	LYS	C	95	99.438	95.590	214.340	1.00	88.70	C
ATOM	4390	N	SER	C	96	98.485	95.550	212.295	1.00	91.18	C
ATOM	4391	CA	SER	C	96	99.688	95.846	211.527	1.00	91.60	C
ATOM	4392	CB	SER	C	96	99.590	95.171	210.154	1.00	92.40	C
ATOM	4393	OG	SER	C	96	98.391	95.534	209.483	1.00	90.75	C
ATOM	4394	C	SER	C	96	99.984	97.337	211.334	1.00	91.57	C
ATOM	4395	O	SER	C	96	101.149	97.740	211.290	1.00	92.99	C
ATOM	4396	N	LYS	C	97	98.941	98.153	211.203	1.00	89.94	C
ATOM	4397	CA	LYS	C	97	99.130	99.590	211.008	1.00	89.77	C
ATOM	4398	CB	LYS	C	97	98.245	100.095	209.864	1.00	91.96	C
ATOM	4399	CG	LYS	C	97	98.266	99.232	208.601	1.00	96.47	C
ATOM	4400	CD	LYS	C	97	99.650	99.129	207.984	1.00	101.18	C
ATOM	4401	CE	LYS	C	97	99.629	98.229	206.757	1.00	102.44	C
ATOM	4402	NZ	LYS	C	97	100.994	97.999	206.207	1.00	104.46	C
ATOM	4403	C	LYS	C	97	98.782	100.337	212.287	1.00	87.93	C
ATOM	4404	O	LYS	C	97	98.601	101.552	212.285	1.00	88.12	C
ATOM	4405	N	LEU	C	98	98.711	99.585	213.377	1.00	87.66	C
ATOM	4406	CA	LEU	C	98	98.367	100.096	214.700	1.00	88.51	C
ATOM	4407	CB	LEU	C	98	98.568	98.965	215.721	1.00	90.90	C
ATOM	4408	CG	LEU	C	98	98.300	99.175	217.215	1.00	92.39	C
ATOM	4409	CD1	LEU	C	98	99.507	99.824	217.867	1.00	90.36	C
ATOM	4410	CD2	LEU	C	98	97.033	100.006	217.407	1.00	93.94	C
ATOM	4411	C	LEU	C	98	99.069	101.382	215.176	1.00	87.33	C
ATOM	4412	O	LEU	C	98	98.411	102.272	215.724	1.00	86.68	C
ATOM	4413	N	THR	C	99	100.386	101.481	214.981	1.00	85.49	C
ATOM	4414	CA	THR	C	99	101.141	102.667	215.408	1.00	81.70	C
ATOM	4415	CB	THR	C	99	102.546	102.302	215.945	1.00	83.64	C
ATOM	4416	OG1	THR	C	99	103.360	101.821	214.863	1.00	84.13	C
ATOM	4417	CG2	THR	C	99	102.453	101.231	217.036	1.00	80.79	C



ATOM	4418	C	THR	C	99	101.331	103.606	214.230	1.00	79.48	C
ATOM	4419	O	THR	C	99	102.323	104.330	214.143	1.00	77.78	C
ATOM	4420	N	GLU	C	100	100.370	103.578	213.318	1.00	78.70	C
ATOM	4421	CA	GLU	C	100	100.408	104.413	212.132	1.00	76.77	C
ATOM	4422	CB	GLU	C	100	100.483	103.542	210.880	1.00	79.30	C
ATOM	4423	CG	GLU	C	100	101.840	102.911	210.636	1.00	84.62	C
ATOM	4424	CD	GLU	C	100	101.815	101.911	209.496	1.00	85.94	C
ATOM	4425	OE1	GLU	C	100	101.329	102.263	208.399	1.00	88.43	C
ATOM	4426	OE2	GLU	C	100	102.287	100.772	209.701	1.00	88.44	C
ATOM	4427	C	GLU	C	100	99.188	105.305	212.028	1.00	73.28	C
ATOM	4428	O	GLU	C	100	98.172	105.067	212.676	1.00	72.87	C
ATOM	4429	N	ASN	C	101	99.304	106.342	211.209	1.00	70.85	C
ATOM	4430	CA	ASN	C	101	98.199	107.250	210.971	1.00	68.56	C
ATOM	4431	CB	ASN	C	101	98.721	108.602	210.512	1.00	68.80	C
ATOM	4432	CG	ASN	C	101	98.890	109.561	211.660	1.00	74.73	C
ATOM	4433	OD1	ASN	C	101	99.057	109.144	212.812	1.00	74.69	C
ATOM	4434	ND2	ASN	C	101	98.851	110.855	211.362	1.00	77.18	C
ATOM	4435	C	ASN	C	101	97.400	106.583	209.876	1.00	66.16	C
ATOM	4436	O	ASN	C	101	97.882	106.436	208.751	1.00	65.12	C
ATOM	4437	N	THR	C	102	96.181	106.171	210.205	1.00	62.42	C
ATOM	4438	CA	THR	C	102	95.347	105.470	209.240	1.00	60.02	C
ATOM	4439	CB	THR	C	102	95.221	103.995	209.626	1.00	61.43	C
ATOM	4440	OG1	THR	C	102	94.630	103.897	210.926	1.00	65.81	C
ATOM	4441	CG2	THR	C	102	96.590	103.336	209.658	1.00	67.01	C
ATOM	4442	C	THR	C	102	93.938	106.000	209.026	1.00	55.44	C
ATOM	4443	O	THR	C	102	93.391	106.748	209.841	1.00	49.92	C
ATOM	4444	N	LEU	C	103	93.369	105.607	207.893	1.00	54.74	C
ATOM	4445	CA	LEU	C	103	91.997	105.971	207.550	1.00	53.90	C
ATOM	4446	CB	LEU	C	103	91.918	107.010	206.426	1.00	49.57	C
ATOM	4447	CG	LEU	C	103	90.470	107.181	205.929	1.00	50.56	C
ATOM	4448	CD1	LEU	C	103	89.617	107.820	207.034	1.00	49.66	C
ATOM	4449	CD2	LEU	C	103	90.435	108.027	204.680	1.00	49.68	C
ATOM	4450	C	LEU	C	103	91.287	104.724	207.069	1.00	50.03	C
ATOM	4451	O	LEU	C	103	91.750	104.053	206.150	1.00	46.64	C
ATOM	4452	N	GLN	C	104	90.173	104.398	207.703	1.00	49.55	C
ATOM	4453	CA	GLN	C	104	89.421	103.243	207.260	1.00	50.66	C
ATOM	4454	CB	GLN	C	104	89.319	102.193	208.366	1.00	50.09	C
ATOM	4455	CG	GLN	C	104	90.127	100.949	208.037	1.00	47.02	C
ATOM	4456	CD	GLN	C	104	89.953	99.844	209.050	1.00	44.86	C
ATOM	4457	OE1	GLN	C	104	90.494	98.757	208.882	1.00	44.24	C
ATOM	4458	NE2	GLN	C	104	89.198	100.115	210.109	1.00	43.43	C
ATOM	4459	C	GLN	C	104	88.038	103.655	206.792	1.00	47.86	C
ATOM	4460	O	GLN	C	104	87.403	104.538	207.378	1.00	45.75	C
ATOM	4461	N	LEU	C	105	87.590	103.031	205.714	1.00	41.37	C
ATOM	4462	CA	LEU	C	105	86.279	103.327	205.198	1.00	39.67	C
ATOM	4463	CB	LEU	C	105	86.339	103.572	203.699	1.00	41.36	C
ATOM	4464	CG	LEU	C	105	87.166	104.767	203.233	1.00	40.66	C
ATOM	4465	CD1	LEU	C	105	86.997	104.929	201.736	1.00	45.24	C
ATOM	4466	CD2	LEU	C	105	86.708	106.027	203.944	1.00	44.36	C
ATOM	4467	C	LEU	C	105	85.369	102.148	205.479	1.00	38.36	C
ATOM	4468	O	LEU	C	105	85.825	101.023	205.609	1.00	40.09	C
ATOM	4469	N	ALA	C	106	84.081	102.429	205.608	1.00	35.79	C
ATOM	4470	CA	ALA	C	106	83.067	101.413	205.837	1.00	28.97	C
ATOM	4471	CB	ALA	C	106	82.457	101.562	207.222	1.00	29.44	C
ATOM	4472	C	ALA	C	106	82.023	101.690	204.767	1.00	28.76	C
ATOM	4473	O	ALA	C	106	81.307	102.704	204.810	1.00	32.17	C
ATOM	4474	N	ILE	C	107	81.951	100.808	203.785	1.00	26.90	C
ATOM	4475	CA	ILE	C	107	80.997	100.995	202.706	1.00	24.23	C



ATOM	4476	CB	ILE	C	107	81.373	100.155	201.487	1.00	24.81	C
ATOM	4477	CG2	ILE	C	107	80.588	100.645	200.257	1.00	23.07	C
ATOM	4478	CG1	ILE	C	107	82.875	100.284	201.217	1.00	21.30	C
ATOM	4479	CD1	ILE	C	107	83.303	101.668	200.752	1.00	20.95	C
ATOM	4480	C	ILE	C	107	79.625	100.573	203.178	1.00	26.48	C
ATOM	4481	O	ILE	C	107	79.483	99.587	203.907	1.00	29.41	C
ATOM	4482	N	ILE	C	108	78.614	101.322	202.762	1.00	25.57	C
ATOM	4483	CA	ILE	C	108	77.245	101.015	203.132	1.00	29.03	C
ATOM	4484	CB	ILE	C	108	76.690	102.055	204.127	1.00	31.74	C
ATOM	4485	CG2	ILE	C	108	75.282	101.650	204.577	1.00	23.26	C
ATOM	4486	CG1	ILE	C	108	77.655	102.210	205.308	1.00	27.10	C
ATOM	4487	CD1	ILE	C	108	77.360	103.432	206.149	1.00	20.06	C
ATOM	4488	C	ILE	C	108	76.394	101.083	201.877	1.00	28.55	C
ATOM	4489	O	ILE	C	108	76.633	101.924	201.015	1.00	27.49	C
ATOM	4490	N	SER	C	109	75.413	100.193	201.764	1.00	27.78	C
ATOM	4491	CA	SER	C	109	74.514	100.238	200.612	1.00	29.78	C
ATOM	4492	CB	SER	C	109	74.409	98.866	199.939	1.00	29.22	C
ATOM	4493	OG	SER	C	109	75.687	98.377	199.544	1.00	30.92	C
ATOM	4494	C	SER	C	109	73.180	100.657	201.226	1.00	31.26	C
ATOM	4495	O	SER	C	109	72.744	100.073	202.225	1.00	33.37	C
ATOM	4496	N	ARG	C	110	72.572	101.700	200.670	1.00	25.46	C
ATOM	4497	CA	ARG	C	110	71.305	102.210	201.170	1.00	28.53	C
ATOM	4498	CB	ARG	C	110	71.449	103.649	201.705	1.00	23.33	C
ATOM	4499	CG	ARG	C	110	70.198	104.509	201.477	1.00	27.53	C
ATOM	4500	CD	ARG	C	110	70.286	105.913	202.073	1.00	23.03	C
ATOM	4501	NE	ARG	C	110	70.324	105.822	203.523	1.00	32.98	C
ATOM	4502	CZ	ARG	C	110	69.476	106.416	204.357	1.00	31.72	C
ATOM	4503	NH1	ARG	C	110	68.490	107.186	203.914	1.00	20.17	C
ATOM	4504	NH2	ARG	C	110	69.601	106.191	205.654	1.00	27.52	C
ATOM	4505	C	ARG	C	110	70.305	102.195	200.024	1.00	34.31	C
ATOM	4506	O	ARG	C	110	70.468	102.909	199.028	1.00	33.63	C
ATOM	4507	N	ILE	C	111	69.258	101.389	200.181	1.00	35.76	C
ATOM	4508	CA	ILE	C	111	68.241	101.269	199.158	1.00	29.74	C
ATOM	4509	CB	ILE	C	111	68.312	99.895	198.520	1.00	30.13	C
ATOM	4510	CG2	ILE	C	111	69.689	99.711	197.867	1.00	30.10	C
ATOM	4511	CG1	ILE	C	111	68.060	98.827	199.581	1.00	27.37	C
ATOM	4512	CD1	ILE	C	111	67.937	97.426	199.020	1.00	26.04	C
ATOM	4513	C	ILE	C	111	66.834	101.504	199.668	1.00	25.68	C
ATOM	4514	O	ILE	C	111	66.549	101.342	200.843	1.00	25.24	C
ATOM	4515	N	LYS	C	112	65.944	101.879	198.768	1.00	23.97	C
ATOM	4516	CA	LYS	C	112	64.575	102.132	199.162	1.00	27.13	C
ATOM	4517	CB	LYS	C	112	63.800	102.802	198.030	1.00	23.28	C
ATOM	4518	CG	LYS	C	112	64.511	103.936	197.346	1.00	24.02	C
ATOM	4519	CD	LYS	C	112	63.679	104.395	196.163	1.00	34.80	C
ATOM	4520	CE	LYS	C	112	64.368	105.466	195.358	1.00	44.00	C
ATOM	4521	NZ	LYS	C	112	63.540	105.871	194.193	1.00	46.30	C
ATOM	4522	C	LYS	C	112	63.867	100.827	199.526	1.00	26.75	C
ATOM	4523	O	LYS	C	112	64.128	99.772	198.965	1.00	26.76	C
ATOM	4524	N	LEU	C	113	62.967	100.921	200.481	1.00	26.13	C
ATOM	4525	CA	LEU	C	113	62.186	99.790	200.911	1.00	29.40	C
ATOM	4526	CB	LEU	C	113	62.617	99.347	202.305	1.00	27.31	C
ATOM	4527	CG	LEU	C	113	61.661	98.419	203.055	1.00	27.04	C
ATOM	4528	CD1	LEU	C	113	61.033	97.429	202.099	1.00	42.12	C
ATOM	4529	CD2	LEU	C	113	62.431	97.669	204.118	1.00	29.99	C
ATOM	4530	C	LEU	C	113	60.770	100.333	200.946	1.00	33.39	C
ATOM	4531	O	LEU	C	113	60.496	101.282	201.682	1.00	40.52	C
ATOM	4532	N	TYR	C	114	59.880	99.789	200.122	1.00	29.57	C
ATOM	4533	CA	TYR	C	114	58.508	100.273	200.151	1.00	32.86	C



ATOM	4534	CB	TYR	C	114	57.930	100.481	198.748	1.00	30.74	C
ATOM	4535	CG	TYR	C	114	58.650	101.478	197.892	1.00	29.60	C
ATOM	4536	CD1	TYR	C	114	59.406	101.062	196.802	1.00	26.10	C
ATOM	4537	CE1	TYR	C	114	60.068	101.969	196.014	1.00	23.29	C
ATOM	4538	CD2	TYR	C	114	58.574	102.838	198.163	1.00	29.47	C
ATOM	4539	CE2	TYR	C	114	59.235	103.761	197.368	1.00	26.92	C
ATOM	4540	CZ	TYR	C	114	59.979	103.319	196.299	1.00	26.65	C
ATOM	4541	OH	TYR	C	114	60.642	104.224	195.506	1.00	33.22	C
ATOM	4542	C	TYR	C	114	57.605	99.298	200.880	1.00	34.84	C
ATOM	4543	O	TYR	C	114	57.677	98.078	200.679	1.00	34.64	C
ATOM	4544	N	TYR	C	115	56.765	99.846	201.743	1.00	35.45	C
ATOM	4545	CA	TYR	C	115	55.786	99.056	202.463	1.00	39.69	C
ATOM	4546	CB	TYR	C	115	55.482	99.703	203.815	1.00	41.42	C
ATOM	4547	CG	TYR	C	115	54.400	99.007	204.590	1.00	45.34	C
ATOM	4548	CD1	TYR	C	115	54.647	97.784	205.211	1.00	47.77	C
ATOM	4549	CE1	TYR	C	115	53.655	97.124	205.925	1.00	48.10	C
ATOM	4550	CD2	TYR	C	115	53.120	99.561	204.699	1.00	46.27	C
ATOM	4551	CE2	TYR	C	115	52.117	98.906	205.412	1.00	47.07	C
ATOM	4552	CZ	TYR	C	115	52.393	97.687	206.023	1.00	48.41	C
ATOM	4553	OH	TYR	C	115	51.416	97.026	206.733	1.00	53.80	C
ATOM	4554	C	TYR	C	115	54.593	99.218	201.524	1.00	41.45	C
ATOM	4555	O	TYR	C	115	54.052	100.313	201.395	1.00	42.19	C
ATOM	4556	N	ARG	C	116	54.205	98.149	200.841	1.00	46.96	C
ATOM	4557	CA	ARG	C	116	53.091	98.229	199.906	1.00	48.56	C
ATOM	4558	CB	ARG	C	116	53.478	97.573	198.582	1.00	50.98	C
ATOM	4559	CG	ARG	C	116	52.379	97.607	197.515	1.00	56.25	C
ATOM	4560	CD	ARG	C	116	52.923	97.169	196.160	1.00	51.16	C
ATOM	4561	NE	ARG	C	116	53.861	98.154	195.633	1.00	53.13	C
ATOM	4562	CZ	ARG	C	116	54.795	97.888	194.726	1.00	48.89	C
ATOM	4563	NH1	ARG	C	116	54.912	96.662	194.248	1.00	46.77	C
ATOM	4564	NH2	ARG	C	116	55.612	98.845	194.300	1.00	46.98	C
ATOM	4565	C	ARG	C	116	51.832	97.583	200.447	1.00	51.42	C
ATOM	4566	O	ARG	C	116	51.708	96.360	200.453	1.00	54.30	C
ATOM	4567	N	PRO	C	117	50.879	98.398	200.917	1.00	56.53	C
ATOM	4568	CD	PRO	C	117	50.852	99.871	200.908	1.00	58.77	C
ATOM	4569	CA	PRO	C	117	49.627	97.859	201.456	1.00	62.45	C
ATOM	4570	CB	PRO	C	117	48.755	99.101	201.625	1.00	60.03	C
ATOM	4571	CG	PRO	C	117	49.747	100.174	201.892	1.00	58.16	C
ATOM	4572	C	PRO	C	117	49.044	96.903	200.435	1.00	66.70	C
ATOM	4573	O	PRO	C	117	48.544	97.330	199.406	1.00	69.54	C
ATOM	4574	N	ALA	C	118	49.134	95.610	200.703	1.00	73.31	C
ATOM	4575	CA	ALA	C	118	48.602	94.623	199.776	1.00	79.41	C
ATOM	4576	CB	ALA	C	118	49.093	93.219	200.164	1.00	83.73	C
ATOM	4577	C	ALA	C	118	47.076	94.689	199.811	1.00	80.96	C
ATOM	4578	O	ALA	C	118	46.447	94.014	200.628	1.00	82.02	C
ATOM	4579	N	LYS	C	119	46.494	95.506	198.928	1.00	81.32	C
ATOM	4580	CA	LYS	C	119	45.041	95.682	198.853	1.00	80.16	C
ATOM	4581	CB	LYS	C	119	44.473	95.911	200.257	1.00	80.43	C
ATOM	4582	CG	LYS	C	119	42.987	95.611	200.409	1.00	82.71	C
ATOM	4583	CD	LYS	C	119	42.715	94.117	200.551	1.00	81.14	C
ATOM	4584	CE	LYS	C	119	41.288	93.868	201.047	1.00	84.48	C
ATOM	4585	NZ	LYS	C	119	40.998	92.436	201.358	1.00	83.97	C
ATOM	4586	C	LYS	C	119	44.686	96.887	197.974	1.00	79.67	C
ATOM	4587	O	LYS	C	119	43.573	97.417	198.043	1.00	79.79	C
ATOM	4588	N	LEU	C	120	45.630	97.315	197.144	1.00	78.27	C
ATOM	4589	CA	LEU	C	120	45.413	98.469	196.280	1.00	77.14	C
ATOM	4590	CB	LEU	C	120	46.727	99.228	196.103	1.00	77.38	C
ATOM	4591	CG	LEU	C	120	47.530	99.426	197.393	1.00	76.41	C



ATOM	4592	CD1	LEU	C	120	48.829	100.148	197.083	1.00	75.66	C
ATOM	4593	CD2	LEU	C	120	46.705	100.200	198.407	1.00	72.90	C
ATOM	4594	C	LEU	C	120	44.856	98.067	194.919	1.00	77.03	C
ATOM	4595	O	LEU	C	120	45.129	96.975	194.415	1.00	76.76	C
ATOM	4596	N	ALA	C	121	44.078	98.965	194.322	1.00	76.76	C
ATOM	4597	CA	ALA	C	121	43.458	98.707	193.025	1.00	73.80	C
ATOM	4598	CB	ALA	C	121	42.311	99.680	192.800	1.00	73.47	C
ATOM	4599	C	ALA	C	121	44.441	98.799	191.872	1.00	71.28	C
ATOM	4600	O	ALA	C	121	44.807	97.796	191.269	1.00	71.09	C
ATOM	4601	N	LEU	C	122	44.863	100.016	191.569	1.00	69.82	C
ATOM	4602	CA	LEU	C	122	45.788	100.244	190.477	1.00	68.48	C
ATOM	4603	CB	LEU	C	122	46.162	101.725	190.431	1.00	65.97	C
ATOM	4604	CG	LEU	C	122	47.332	102.127	189.535	1.00	67.82	C
ATOM	4605	CD1	LEU	C	122	47.306	101.337	188.240	1.00	68.18	C
ATOM	4606	CD2	LEU	C	122	47.259	103.624	189.274	1.00	69.44	C
ATOM	4607	C	LEU	C	122	47.041	99.390	190.576	1.00	68.66	C
ATOM	4608	O	LEU	C	122	47.872	99.606	191.440	1.00	71.50	C
ATOM	4609	N	PRO	C	123	47.195	98.407	189.680	1.00	70.18	C
ATOM	4610	CD	PRO	C	123	46.281	98.031	188.586	1.00	72.27	C
ATOM	4611	CA	PRO	C	123	48.375	97.536	189.698	1.00	71.13	C
ATOM	4612	CB	PRO	C	123	47.993	96.432	188.714	1.00	72.33	C
ATOM	4613	CG	PRO	C	123	47.168	97.168	187.700	1.00	72.84	C
ATOM	4614	C	PRO	C	123	49.655	98.286	189.293	1.00	70.11	C
ATOM	4615	O	PRO	C	123	49.688	98.984	188.277	1.00	69.35	C
ATOM	4616	N	PRO	C	124	50.728	98.130	190.082	1.00	68.55	C
ATOM	4617	CD	PRO	C	124	50.843	97.097	191.121	1.00	66.12	C
ATOM	4618	CA	PRO	C	124	52.027	98.773	189.857	1.00	68.08	C
ATOM	4619	CB	PRO	C	124	53.002	97.882	190.638	1.00	66.35	C
ATOM	4620	CG	PRO	C	124	52.235	96.619	190.898	1.00	68.45	C
ATOM	4621	C	PRO	C	124	52.449	98.992	188.407	1.00	67.98	C
ATOM	4622	O	PRO	C	124	52.988	100.040	188.059	1.00	66.69	C
ATOM	4623	N	ASP	C	125	52.211	98.004	187.564	1.00	70.69	C
ATOM	4624	CA	ASP	C	125	52.562	98.111	186.152	1.00	76.00	C
ATOM	4625	CB	ASP	C	125	52.093	96.860	185.433	1.00	82.61	C
ATOM	4626	CG	ASP	C	125	50.626	96.577	185.692	1.00	90.11	C
ATOM	4627	OD1	ASP	C	125	49.761	97.326	185.181	1.00	92.24	C
ATOM	4628	OD2	ASP	C	125	50.336	95.613	186.429	1.00	95.35	C
ATOM	4629	C	ASP	C	125	51.869	99.312	185.515	1.00	76.82	C
ATOM	4630	O	ASP	C	125	52.426	99.993	184.653	1.00	76.53	C
ATOM	4631	N	GLN	C	126	50.644	99.554	185.964	1.00	76.65	C
ATOM	4632	CA	GLN	C	126	49.791	100.615	185.451	1.00	77.88	C
ATOM	4633	CB	GLN	C	126	48.345	100.086	185.509	1.00	84.26	C
ATOM	4634	CG	GLN	C	126	47.238	100.918	184.851	1.00	90.11	C
ATOM	4635	CD	GLN	C	126	45.876	100.222	184.942	1.00	91.50	C
ATOM	4636	OE1	GLN	C	126	44.827	100.834	184.711	1.00	90.64	C
ATOM	4637	NE2	GLN	C	126	45.895	98.931	185.277	1.00	90.61	C
ATOM	4638	C	GLN	C	126	49.933	101.953	186.202	1.00	76.75	C
ATOM	4639	O	GLN	C	126	48.961	102.698	186.342	1.00	76.79	C
ATOM	4640	N	ALA	C	127	51.143	102.275	186.661	1.00	72.89	C
ATOM	4641	CA	ALA	C	127	51.351	103.516	187.408	1.00	67.15	C
ATOM	4642	CB	ALA	C	127	52.056	103.214	188.714	1.00	62.36	C
ATOM	4643	C	ALA	C	127	52.086	104.633	186.664	1.00	65.58	C
ATOM	4644	O	ALA	C	127	51.665	105.784	186.707	1.00	65.29	C
ATOM	4645	N	ALA	C	128	53.176	104.307	185.981	1.00	64.51	C
ATOM	4646	CA	ALA	C	128	53.934	105.323	185.259	1.00	66.86	C
ATOM	4647	CB	ALA	C	128	55.050	104.668	184.455	1.00	62.32	C
ATOM	4648	C	ALA	C	128	53.053	106.173	184.338	1.00	71.69	C
ATOM	4649	O	ALA	C	128	53.219	107.393	184.266	1.00	72.64	C



ATOM	4650	N	GLU	C	129	52.116	105.527	183.645	1.00	74.88	C
ATOM	4651	CA	GLU	C	129	51.210	106.211	182.719	1.00	76.58	C
ATOM	4652	CB	GLU	C	129	50.205	105.228	182.140	1.00	82.30	C
ATOM	4653	CG	GLU	C	129	50.659	103.782	182.161	1.00	99.89	C
ATOM	4654	CD	GLU	C	129	49.483	102.811	182.147	1.00	105.74	C
ATOM	4655	OE1	GLU	C	129	49.718	101.593	181.954	1.00	108.41	C
ATOM	4656	OE2	GLU	C	129	48.329	103.270	182.341	1.00	107.68	C
ATOM	4657	C	GLU	C	129	50.416	107.315	183.402	1.00	76.13	C
ATOM	4658	O	GLU	C	129	50.218	108.394	182.839	1.00	78.21	C
ATOM	4659	N	LYS	C	130	49.941	107.026	184.609	1.00	71.78	C
ATOM	4660	CA	LYS	C	130	49.137	107.971	185.372	1.00	68.78	C
ATOM	4661	CB	LYS	C	130	48.663	107.317	186.671	1.00	73.45	C
ATOM	4662	CG	LYS	C	130	47.932	105.988	186.491	1.00	76.44	C
ATOM	4663	CD	LYS	C	130	46.565	106.174	185.855	1.00	77.83	C
ATOM	4664	CE	LYS	C	130	45.892	104.842	185.572	1.00	80.13	C
ATOM	4665	NZ	LYS	C	130	44.536	105.033	184.979	1.00	81.02	C
ATOM	4666	C	LYS	C	130	49.880	109.254	185.706	1.00	66.73	C
ATOM	4667	O	LYS	C	130	49.310	110.162	186.309	1.00	65.89	C
ATOM	4668	N	LEU	C	131	51.146	109.333	185.312	1.00	66.23	C
ATOM	4669	CA	LEU	C	131	51.959	110.506	185.602	1.00	67.46	C
ATOM	4670	CB	LEU	C	131	53.446	110.179	185.460	1.00	61.90	C
ATOM	4671	CG	LEU	C	131	54.348	111.322	185.948	1.00	59.71	C
ATOM	4672	CD1	LEU	C	131	54.235	111.422	187.477	1.00	51.94	C
ATOM	4673	CD2	LEU	C	131	55.789	111.094	185.519	1.00	52.03	C
ATOM	4674	C	LEU	C	131	51.651	111.704	184.726	1.00	72.09	C
ATOM	4675	O	LEU	C	131	52.006	111.723	183.547	1.00	77.45	C
ATOM	4676	N	ARG	C	132	51.009	112.713	185.302	1.00	75.62	C
ATOM	4677	CA	ARG	C	132	50.685	113.924	184.554	1.00	81.97	C
ATOM	4678	CB	ARG	C	132	49.296	114.425	184.948	1.00	86.32	C
ATOM	4679	CG	ARG	C	132	48.203	113.376	184.812	1.00	94.44	C
ATOM	4680	CD	ARG	C	132	46.949	113.787	185.582	1.00	101.07	C
ATOM	4681	NE	ARG	C	132	46.076	112.648	185.869	1.00	105.90	C
ATOM	4682	CZ	ARG	C	132	45.035	112.688	186.700	1.00	106.82	C
ATOM	4683	NH1	ARG	C	132	44.724	113.814	187.334	1.00	104.57	C
ATOM	4684	NH2	ARG	C	132	44.313	111.594	186.909	1.00	107.65	C
ATOM	4685	C	ARG	C	132	51.738	114.991	184.854	1.00	83.29	C
ATOM	4686	O	ARG	C	132	52.732	114.716	185.529	1.00	81.71	C
ATOM	4687	N	PHE	C	133	51.530	116.205	184.354	1.00	85.41	C
ATOM	4688	CA	PHE	C	133	52.487	117.280	184.585	1.00	89.36	C
ATOM	4689	CB	PHE	C	133	53.489	117.352	183.431	1.00	89.20	C
ATOM	4690	CG	PHE	C	133	54.402	116.167	183.348	1.00	90.91	C
ATOM	4691	CD1	PHE	C	133	53.928	114.934	182.914	1.00	91.02	C
ATOM	4692	CD2	PHE	C	133	55.737	116.278	183.726	1.00	92.17	C
ATOM	4693	CE1	PHE	C	133	54.768	113.827	182.861	1.00	92.37	C
ATOM	4694	CE2	PHE	C	133	56.591	115.180	183.678	1.00	90.72	C
ATOM	4695	CZ	PHE	C	133	56.105	113.949	183.244	1.00	91.94	C
ATOM	4696	C	PHE	C	133	51.875	118.665	184.799	1.00	92.81	C
ATOM	4697	O	PHE	C	133	50.684	118.809	185.085	1.00	94.77	C
ATOM	4698	N	ARG	C	134	52.723	119.677	184.661	1.00	94.38	C
ATOM	4699	CA	ARG	C	134	52.354	121.078	184.825	1.00	97.15	C
ATOM	4700	CB	ARG	C	134	51.895	121.351	186.252	1.00	94.06	C
ATOM	4701	CG	ARG	C	134	51.710	122.820	186.566	1.00	95.15	C
ATOM	4702	CD	ARG	C	134	51.724	123.035	188.066	1.00	99.61	C
ATOM	4703	NE	ARG	C	134	50.655	122.292	188.727	1.00	102.22	C
ATOM	4704	CZ	ARG	C	134	50.652	121.984	190.020	1.00	102.69	C
ATOM	4705	NH1	ARG	C	134	51.669	122.352	190.793	1.00	101.46	C
ATOM	4706	NH2	ARG	C	134	49.630	121.312	190.542	1.00	101.62	C
ATOM	4707	C	ARG	C	134	53.644	121.836	184.551	1.00	101.12	C



ATOM	4708	O	ARG	C	134	54.426	122.108	185.467	1.00101.67	C
ATOM	4709	N	ARG	C	135	53.861	122.181	183.286	1.00103.95	C
ATOM	4710	CA	ARG	C	135	55.090	122.853	182.890	1.00105.02	C
ATOM	4711	CB	ARG	C	135	55.636	122.184	181.634	1.00105.65	C
ATOM	4712	CG	ARG	C	135	54.808	122.423	180.392	1.00104.70	C
ATOM	4713	CD	ARG	C	135	55.623	123.246	179.441	1.00106.30	C
ATOM	4714	NE	ARG	C	135	56.926	122.623	179.262	1.00106.12	C
ATOM	4715	CZ	ARG	C	135	58.007	123.255	178.827	1.00106.19	C
ATOM	4716	NH1	ARG	C	135	59.148	122.591	178.698	1.00107.56	C
ATOM	4717	NH2	ARG	C	135	57.951	124.547	178.530	1.00105.16	C
ATOM	4718	C	ARG	C	135	55.022	124.353	182.659	1.00105.53	C
ATOM	4719	O	ARG	C	135	54.334	124.816	181.750	1.00106.67	C
ATOM	4720	N	SER	C	136	55.747	125.105	183.485	1.00105.05	C
ATOM	4721	CA	SER	C	136	55.811	126.559	183.360	1.00105.50	C
ATOM	4722	CB	SER	C	136	55.920	127.222	184.740	1.00104.11	C
ATOM	4723	OG	SER	C	136	54.696	127.143	185.449	1.00103.41	C
ATOM	4724	C	SER	C	136	57.050	126.889	182.527	1.00106.70	C
ATOM	4725	O	SER	C	136	57.347	126.200	181.548	1.00107.30	C
ATOM	4726	N	ALA	C	137	57.768	127.939	182.908	1.00107.29	C
ATOM	4727	CA	ALA	C	137	58.984	128.325	182.199	1.00107.41	C
ATOM	4728	CB	ALA	C	137	58.876	129.762	181.719	1.00106.98	C
ATOM	4729	C	ALA	C	137	60.146	128.177	183.173	1.00107.82	C
ATOM	4730	O	ALA	C	137	61.259	128.646	182.918	1.00106.77	C
ATOM	4731	N	ASN	C	138	59.864	127.513	184.293	1.00108.40	C
ATOM	4732	CA	ASN	C	138	60.849	127.293	185.344	1.00107.89	C
ATOM	4733	CB	ASN	C	138	61.174	128.623	186.034	1.00108.60	C
ATOM	4734	CG	ASN	C	138	59.925	129.434	186.376	1.00109.12	C
ATOM	4735	OD1	ASN	C	138	59.013	128.961	187.070	1.00105.10	C
ATOM	4736	ND2	ASN	C	138	59.885	130.667	185.885	1.00106.89	C
ATOM	4737	C	ASN	C	138	60.396	126.284	186.398	1.00105.81	C
ATOM	4738	O	ASN	C	138	61.217	125.727	187.125	1.00104.03	C
ATOM	4739	N	SER	C	139	59.094	126.033	186.471	1.00104.30	C
ATOM	4740	CA	SER	C	139	58.584	125.120	187.483	1.00101.96	C
ATOM	4741	CB	SER	C	139	57.818	125.927	188.533	1.00101.41	C
ATOM	4742	OG	SER	C	139	58.575	127.050	188.956	1.00102.22	C
ATOM	4743	C	SER	C	139	57.714	123.960	186.993	1.00100.89	C
ATOM	4744	O	SER	C	139	56.491	123.978	187.162	1.00101.72	C
ATOM	4745	N	LEU	C	140	58.346	122.951	186.394	1.00 97.77	C
ATOM	4746	CA	LEU	C	140	57.629	121.767	185.922	1.00 92.68	C
ATOM	4747	CB	LEU	C	140	58.515	120.957	184.983	1.00 90.35	C
ATOM	4748	CG	LEU	C	140	57.815	119.856	184.185	1.00 91.97	C
ATOM	4749	CD1	LEU	C	140	58.850	119.104	183.349	1.00 89.68	C
ATOM	4750	CD2	LEU	C	140	57.083	118.909	185.125	1.00 90.76	C
ATOM	4751	C	LEU	C	140	57.314	120.942	187.172	1.00 90.20	C
ATOM	4752	O	LEU	C	140	58.211	120.599	187.938	1.00 92.58	C
ATOM	4753	N	THR	C	141	56.049	120.603	187.372	1.00 85.90	C
ATOM	4754	CA	THR	C	141	55.664	119.867	188.567	1.00 83.10	C
ATOM	4755	CB	THR	C	141	54.619	120.683	189.373	1.00 82.55	C
ATOM	4756	OG1	THR	C	141	55.171	121.966	189.691	1.00 82.12	C
ATOM	4757	CG2	THR	C	141	54.231	119.960	190.669	1.00 81.52	C
ATOM	4758	C	THR	C	141	55.129	118.450	188.362	1.00 82.39	C
ATOM	4759	O	THR	C	141	53.925	118.260	188.149	1.00 82.43	C
ATOM	4760	N	LEU	C	142	56.023	117.461	188.450	1.00 77.27	C
ATOM	4761	CA	LEU	C	142	55.637	116.057	188.307	1.00 71.84	C
ATOM	4762	CB	LEU	C	142	56.790	115.130	188.707	1.00 66.72	C
ATOM	4763	CG	LEU	C	142	58.185	115.145	188.052	1.00 69.00	C
ATOM	4764	CD1	LEU	C	142	58.160	114.463	186.701	1.00 63.82	C
ATOM	4765	CD2	LEU	C	142	58.699	116.572	187.944	1.00 67.43	C



ATOM	4766	C	LEU	C	142	54.461	115.834	189.259	1.00	72.11	C
ATOM	4767	O	LEU	C	142	54.493	116.273	190.408	1.00	70.94	C
ATOM	4768	N	ILE	C	143	53.417	115.167	188.781	1.00	72.83	C
ATOM	4769	CA	ILE	C	143	52.244	114.918	189.609	1.00	72.56	C
ATOM	4770	CB	ILE	C	143	51.070	115.823	189.170	1.00	73.87	C
ATOM	4771	CG2	ILE	C	143	51.135	116.059	187.680	1.00	75.28	C
ATOM	4772	CG1	ILE	C	143	49.730	115.210	189.586	1.00	72.87	C
ATOM	4773	CD1	ILE	C	143	49.495	115.186	191.084	1.00	77.03	C
ATOM	4774	C	ILE	C	143	51.827	113.457	189.549	1.00	72.54	C
ATOM	4775	O	ILE	C	143	51.469	112.947	188.491	1.00	73.64	C
ATOM	4776	N	ASN	C	144	51.872	112.795	190.702	1.00	72.15	C
ATOM	4777	CA	ASN	C	144	51.524	111.379	190.812	1.00	69.54	C
ATOM	4778	CB	ASN	C	144	52.730	110.595	191.346	1.00	67.79	C
ATOM	4779	CG	ASN	C	144	52.398	109.159	191.687	1.00	67.15	C
ATOM	4780	OD1	ASN	C	144	51.335	108.651	191.333	1.00	66.56	C
ATOM	4781	ND2	ASN	C	144	53.320	108.491	192.373	1.00	65.10	C
ATOM	4782	C	ASN	C	144	50.312	111.160	191.709	1.00	67.07	C
ATOM	4783	O	ASN	C	144	50.370	111.395	192.911	1.00	64.81	C
ATOM	4784	N	PRO	C	145	49.192	110.709	191.119	1.00	68.79	C
ATOM	4785	CD	PRO	C	145	48.991	110.730	189.656	1.00	68.70	C
ATOM	4786	CA	PRO	C	145	47.923	110.436	191.804	1.00	68.43	C
ATOM	4787	CB	PRO	C	145	46.896	110.812	190.752	1.00	69.14	C
ATOM	4788	CG	PRO	C	145	47.554	110.264	189.507	1.00	70.72	C
ATOM	4789	C	PRO	C	145	47.748	108.986	192.258	1.00	68.08	C
ATOM	4790	O	PRO	C	145	46.808	108.664	192.986	1.00	69.28	C
ATOM	4791	N	THR	C	146	48.645	108.111	191.820	1.00	67.03	C
ATOM	4792	CA	THR	C	146	48.575	106.699	192.181	1.00	63.58	C
ATOM	4793	CB	THR	C	146	49.526	105.885	191.309	1.00	62.52	C
ATOM	4794	OG1	THR	C	146	50.795	105.778	191.956	1.00	57.38	C
ATOM	4795	CG2	THR	C	146	49.728	106.579	189.970	1.00	64.49	C
ATOM	4796	C	THR	C	146	48.991	106.527	193.635	1.00	64.63	C
ATOM	4797	O	THR	C	146	49.184	107.506	194.348	1.00	68.21	C
ATOM	4798	N	PRO	C	147	49.105	105.280	194.107	1.00	63.48	C
ATOM	4799	CD	PRO	C	147	48.314	104.122	193.655	1.00	66.45	C
ATOM	4800	CA	PRO	C	147	49.515	105.092	195.501	1.00	60.60	C
ATOM	4801	CB	PRO	C	147	48.470	104.133	196.027	1.00	63.08	C
ATOM	4802	CG	PRO	C	147	48.353	103.189	194.872	1.00	66.43	C
ATOM	4803	C	PRO	C	147	50.921	104.505	195.597	1.00	56.95	C
ATOM	4804	O	PRO	C	147	51.264	103.882	196.598	1.00	55.51	C
ATOM	4805	N	TYR	C	148	51.724	104.700	194.554	1.00	54.74	C
ATOM	4806	CA	TYR	C	148	53.096	104.186	194.533	1.00	54.65	C
ATOM	4807	CB	TYR	C	148	53.303	103.179	193.396	1.00	51.56	C
ATOM	4808	CG	TYR	C	148	52.291	102.076	193.318	1.00	55.39	C
ATOM	4809	CD1	TYR	C	148	51.013	102.300	192.805	1.00	54.49	C
ATOM	4810	CE1	TYR	C	148	50.077	101.265	192.740	1.00	54.32	C
ATOM	4811	CD2	TYR	C	148	52.611	100.793	193.762	1.00	59.71	C
ATOM	4812	CE2	TYR	C	148	51.683	99.753	193.703	1.00	57.62	C
ATOM	4813	CZ	TYR	C	148	50.422	99.997	193.195	1.00	55.86	C
ATOM	4814	OH	TYR	C	148	49.510	98.969	193.180	1.00	60.78	C
ATOM	4815	C	TYR	C	148	54.119	105.293	194.337	1.00	52.87	C
ATOM	4816	O	TYR	C	148	53.842	106.300	193.680	1.00	54.93	C
ATOM	4817	N	TYR	C	149	55.308	105.102	194.897	1.00	47.46	C
ATOM	4818	CA	TYR	C	149	56.358	106.087	194.723	1.00	42.87	C
ATOM	4819	CB	TYR	C	149	57.512	105.848	195.709	1.00	41.06	C
ATOM	4820	CG	TYR	C	149	57.335	106.518	197.044	1.00	43.02	C
ATOM	4821	CD1	TYR	C	149	56.552	105.944	198.039	1.00	46.38	C
ATOM	4822	CE1	TYR	C	149	56.341	106.598	199.264	1.00	47.23	C
ATOM	4823	CD2	TYR	C	149	57.911	107.761	197.301	1.00	47.94	C



ATOM	4824	CE2	TYR	C	149	57.705	108.425	198.525	1.00	43.85	C
ATOM	4825	CZ	TYR	C	149	56.921	107.837	199.497	1.00	42.45	C
ATOM	4826	OH	TYR	C	149	56.717	108.471	200.700	1.00	44.06	C
ATOM	4827	C	TYR	C	149	56.862	105.971	193.283	1.00	40.37	C
ATOM	4828	O	TYR	C	149	57.246	104.892	192.829	1.00	40.63	C
ATOM	4829	N	LEU	C	150	56.859	107.080	192.560	1.00	35.91	C
ATOM	4830	CA	LEU	C	150	57.325	107.037	191.194	1.00	36.47	C
ATOM	4831	CB	LEU	C	150	56.410	107.873	190.284	1.00	37.72	C
ATOM	4832	CG	LEU	C	150	54.954	107.390	190.132	1.00	44.89	C
ATOM	4833	CD1	LEU	C	150	54.236	108.267	189.126	1.00	44.46	C
ATOM	4834	CD2	LEU	C	150	54.910	105.929	189.655	1.00	45.28	C
ATOM	4835	C	LEU	C	150	58.748	107.534	191.112	1.00	35.58	C
ATOM	4836	O	LEU	C	150	59.044	108.683	191.461	1.00	34.54	C
ATOM	4837	N	THR	C	151	59.639	106.654	190.674	1.00	35.14	C
ATOM	4838	CA	THR	C	151	61.032	107.029	190.523	1.00	39.49	C
ATOM	4839	CB	THR	C	151	61.992	105.850	190.862	1.00	38.22	C
ATOM	4840	OG1	THR	C	151	61.751	105.396	192.200	1.00	35.24	C
ATOM	4841	CG2	THR	C	151	63.448	106.295	190.753	1.00	37.54	C
ATOM	4842	C	THR	C	151	61.212	107.453	189.070	1.00	43.69	C
ATOM	4843	O	THR	C	151	61.612	106.657	188.219	1.00	45.08	C
ATOM	4844	N	VAL	C	152	60.883	108.712	188.796	1.00	47.76	C
ATOM	4845	CA	VAL	C	152	61.001	109.279	187.459	1.00	52.50	C
ATOM	4846	CB	VAL	C	152	60.224	110.604	187.348	1.00	54.82	C
ATOM	4847	CG1	VAL	C	152	60.549	111.283	186.030	1.00	54.59	C
ATOM	4848	CG2	VAL	C	152	58.726	110.346	187.467	1.00	52.61	C
ATOM	4849	C	VAL	C	152	62.454	109.558	187.116	1.00	54.39	C
ATOM	4850	O	VAL	C	152	63.126	110.304	187.815	1.00	56.59	C
ATOM	4851	N	THR	C	153	62.926	108.954	186.036	1.00	57.56	C
ATOM	4852	CA	THR	C	153	64.293	109.140	185.581	1.00	61.61	C
ATOM	4853	CB	THR	C	153	65.140	107.882	185.881	1.00	62.07	C
ATOM	4854	OG1	THR	C	153	66.503	108.091	185.477	1.00	62.08	C
ATOM	4855	CG2	THR	C	153	64.557	106.675	185.160	1.00	61.10	C
ATOM	4856	C	THR	C	153	64.264	109.423	184.068	1.00	66.39	C
ATOM	4857	O	THR	C	153	63.222	109.264	183.411	1.00	63.99	C
ATOM	4858	N	GLU	C	154	65.406	109.850	183.528	1.00	69.21	C
ATOM	4859	CA	GLU	C	154	65.531	110.189	182.110	1.00	71.00	C
ATOM	4860	CB	GLU	C	154	65.541	108.929	181.249	1.00	68.39	C
ATOM	4861	CG	GLU	C	154	66.776	108.080	181.450	1.00	74.25	C
ATOM	4862	CD	GLU	C	154	67.030	107.138	180.292	1.00	79.00	C
ATOM	4863	OE1	GLU	C	154	68.029	106.383	180.340	1.00	78.01	C
ATOM	4864	OE2	GLU	C	154	66.232	107.160	179.331	1.00	84.26	C
ATOM	4865	C	GLU	C	154	64.419	111.123	181.650	1.00	72.60	C
ATOM	4866	O	GLU	C	154	63.837	110.941	180.581	1.00	73.81	C
ATOM	4867	N	LEU	C	155	64.131	112.127	182.472	1.00	74.75	C
ATOM	4868	CA	LEU	C	155	63.098	113.110	182.168	1.00	77.41	C
ATOM	4869	CB	LEU	C	155	62.668	113.835	183.444	1.00	71.93	C
ATOM	4870	CG	LEU	C	155	61.479	114.787	183.332	1.00	69.10	C
ATOM	4871	CD1	LEU	C	155	60.217	114.000	182.994	1.00	69.43	C
ATOM	4872	CD2	LEU	C	155	61.305	115.530	184.642	1.00	67.56	C
ATOM	4873	C	LEU	C	155	63.672	114.117	181.181	1.00	82.70	C
ATOM	4874	O	LEU	C	155	64.861	114.435	181.237	1.00	83.75	C
ATOM	4875	N	ASN	C	156	62.833	114.620	180.281	1.00	87.15	C
ATOM	4876	CA	ASN	C	156	63.288	115.589	179.294	1.00	89.66	C
ATOM	4877	CB	ASN	C	156	63.842	114.852	178.084	1.00	87.16	C
ATOM	4878	CG	ASN	C	156	64.823	113.775	178.475	1.00	89.41	C
ATOM	4879	OD1	ASN	C	156	65.894	114.063	179.005	1.00	91.24	C
ATOM	4880	ND2	ASN	C	156	64.457	112.522	178.234	1.00	91.32	C
ATOM	4881	C	ASN	C	156	62.181	116.537	178.862	1.00	92.85	C



ATOM	4882	O	ASN	C	156	61.040	116.120	178.643	1.00	90.98	C
ATOM	4883	N	ALA	C	157	62.531	117.816	178.754	1.00	97.40	C
ATOM	4884	CA	ALA	C	157	61.592	118.851	178.334	1.00101.49		C
ATOM	4885	CB	ALA	C	157	62.098	120.222	178.769	1.00101.71		C
ATOM	4886	C	ALA	C	157	61.490	118.784	176.815	1.00104.86		C
ATOM	4887	O	ALA	C	157	61.313	119.799	176.137	1.00106.02		C
ATOM	4888	N	GLY	C	158	61.612	117.566	176.296	1.00107.96		C
ATOM	4889	CA	GLY	C	158	61.554	117.341	174.867	1.00109.79		C
ATOM	4890	C	GLY	C	158	62.939	117.032	174.338	1.00111.23		C
ATOM	4891	O	GLY	C	158	63.175	115.957	173.783	1.00110.98		C
ATOM	4892	N	THR	C	159	63.853	117.983	174.521	1.00113.28		C
ATOM	4893	CA	THR	C	159	65.237	117.848	174.071	1.00115.67		C
ATOM	4894	CB	THR	C	159	65.618	118.953	173.072	1.00116.95		C
ATOM	4895	OG1	THR	C	159	65.539	120.228	173.725	1.00119.65		C
ATOM	4896	CG2	THR	C	159	64.680	118.945	171.870	1.00118.58		C
ATOM	4897	C	THR	C	159	66.148	117.993	175.275	1.00116.35		C
ATOM	4898	O	THR	C	159	67.091	117.222	175.457	1.00116.21		C
ATOM	4899	N	ARG	C	160	65.855	119.001	176.090	1.00116.92		C
ATOM	4900	CA	ARG	C	160	66.627	119.277	177.289	1.00117.75		C
ATOM	4901	CB	ARG	C	160	66.134	120.573	177.940	1.00122.92		C
ATOM	4902	CG	ARG	C	160	66.976	121.059	179.117	1.00131.21		C
ATOM	4903	CD	ARG	C	160	68.270	121.739	178.652	1.00136.40		C
ATOM	4904	NE	ARG	C	160	68.954	122.441	179.738	1.00140.29		C
ATOM	4905	CZ	ARG	C	160	69.755	121.861	180.628	1.00140.43		C
ATOM	4906	NH1	ARG	C	160	69.995	120.554	180.568	1.00141.59		C
ATOM	4907	NH2	ARG	C	160	70.295	122.587	181.600	1.00139.43		C
ATOM	4908	C	ARG	C	160	66.477	118.120	178.272	1.00114.86		C
ATOM	4909	O	ARG	C	160	65.381	117.590	178.465	1.00114.15		C
ATOM	4910	N	VAL	C	161	67.587	117.727	178.883	1.00111.05		C
ATOM	4911	CA	VAL	C	161	67.574	116.646	179.860	1.00107.63		C
ATOM	4912	CB	VAL	C	161	68.840	115.759	179.736	1.00110.07		C
ATOM	4913	CG1	VAL	C	161	70.099	116.601	179.949	1.00110.93		C
ATOM	4914	CG2	VAL	C	161	68.775	114.617	180.742	1.00109.02		C
ATOM	4915	C	VAL	C	161	67.512	117.248	181.260	1.00103.14		C
ATOM	4916	O	VAL	C	161	68.272	118.160	181.592	1.00103.82		C
ATOM	4917	N	LEU	C	162	66.606	116.740	182.084	1.00	97.66	C
ATOM	4918	CA	LEU	C	162	66.462	117.260	183.436	1.00	93.72	C
ATOM	4919	CB	LEU	C	162	64.983	117.495	183.740	1.00	93.66	C
ATOM	4920	CG	LEU	C	162	64.294	118.520	182.843	1.00	91.72	C
ATOM	4921	CD1	LEU	C	162	62.854	118.716	183.294	1.00	88.89	C
ATOM	4922	CD2	LEU	C	162	65.057	119.830	182.911	1.00	90.96	C
ATOM	4923	C	LEU	C	162	67.072	116.390	184.535	1.00	90.67	C
ATOM	4924	O	LEU	C	162	67.895	115.504	184.280	1.00	90.29	C
ATOM	4925	N	GLU	C	163	66.656	116.660	185.765	1.00	86.34	C
ATOM	4926	CA	GLU	C	163	67.147	115.925	186.918	1.00	82.23	C
ATOM	4927	CB	GLU	C	163	67.556	116.915	188.009	1.00	86.91	C
ATOM	4928	CG	GLU	C	163	68.406	116.325	189.114	1.00	94.31	C
ATOM	4929	CD	GLU	C	163	69.333	117.359	189.727	1.00	97.20	C
ATOM	4930	OE1	GLU	C	163	70.339	117.709	189.070	1.00	95.31	C
ATOM	4931	OE2	GLU	C	163	69.049	117.828	190.853	1.00	99.85	C
ATOM	4932	C	GLU	C	163	66.069	114.966	187.420	1.00	75.97	C
ATOM	4933	O	GLU	C	163	64.889	115.325	187.514	1.00	75.64	C
ATOM	4934	N	ASN	C	164	66.487	113.741	187.728	1.00	67.24	C
ATOM	4935	CA	ASN	C	164	65.581	112.698	188.202	1.00	59.92	C
ATOM	4936	CB	ASN	C	164	66.388	111.501	188.675	1.00	59.24	C
ATOM	4937	CG	ASN	C	164	67.443	111.095	187.679	1.00	62.11	C
ATOM	4938	OD1	ASN	C	164	67.134	110.591	186.596	1.00	63.06	C
ATOM	4939	ND2	ASN	C	164	68.702	111.326	188.028	1.00	66.93	C



ATOM	4940	C	ASN	C	164	64.668	113.161	189.326	1.00	56.66	C
ATOM	4941	O	ASN	C	164	64.967	114.114	190.043	1.00	59.30	C
ATOM	4942	N	ALA	C	165	63.548	112.482	189.493	1.00	51.93	C
ATOM	4943	CA	ALA	C	165	62.635	112.864	190.546	1.00	49.65	C
ATOM	4944	CB	ALA	C	165	61.572	113.788	190.003	1.00	52.53	C
ATOM	4945	C	ALA	C	165	61.997	111.641	191.167	1.00	50.47	C
ATOM	4946	O	ALA	C	165	61.908	110.580	190.544	1.00	50.53	C
ATOM	4947	N	LEU	C	166	61.578	111.801	192.415	1.00	46.38	C
ATOM	4948	CA	LEU	C	166	60.923	110.746	193.159	1.00	43.58	C
ATOM	4949	CB	LEU	C	166	61.735	110.397	194.408	1.00	36.70	C
ATOM	4950	CG	LEU	C	166	61.098	109.376	195.357	1.00	44.53	C
ATOM	4951	CD1	LEU	C	166	60.921	108.027	194.636	1.00	36.17	C
ATOM	4952	CD2	LEU	C	166	61.969	109.216	196.586	1.00	33.99	C
ATOM	4953	C	LEU	C	166	59.576	111.337	193.535	1.00	44.39	C
ATOM	4954	O	LEU	C	166	59.487	112.201	194.401	1.00	44.64	C
ATOM	4955	N	VAL	C	167	58.518	110.888	192.874	1.00	45.73	C
ATOM	4956	CA	VAL	C	167	57.213	111.455	193.162	1.00	45.36	C
ATOM	4957	CB	VAL	C	167	56.405	111.732	191.883	1.00	44.90	C
ATOM	4958	CG1	VAL	C	167	55.168	112.544	192.233	1.00	47.30	C
ATOM	4959	CG2	VAL	C	167	57.268	112.470	190.863	1.00	40.79	C
ATOM	4960	C	VAL	C	167	56.377	110.596	194.071	1.00	45.36	C
ATOM	4961	O	VAL	C	167	55.943	109.508	193.710	1.00	48.17	C
ATOM	4962	N	PRO	C	168	56.126	111.098	195.274	1.00	46.56	C
ATOM	4963	CD	PRO	C	168	56.583	112.430	195.704	1.00	44.33	C
ATOM	4964	CA	PRO	C	168	55.341	110.448	196.322	1.00	49.57	C
ATOM	4965	CB	PRO	C	168	55.409	111.454	197.464	1.00	49.44	C
ATOM	4966	CG	PRO	C	168	55.565	112.774	196.747	1.00	49.37	C
ATOM	4967	C	PRO	C	168	53.903	110.122	195.926	1.00	53.61	C
ATOM	4968	O	PRO	C	168	53.306	110.802	195.097	1.00	54.91	C
ATOM	4969	N	PRO	C	169	53.329	109.069	196.528	1.00	56.47	C
ATOM	4970	CD	PRO	C	169	54.009	108.184	197.488	1.00	60.09	C
ATOM	4971	CA	PRO	C	169	51.961	108.602	196.288	1.00	58.83	C
ATOM	4972	CB	PRO	C	169	51.789	107.495	197.323	1.00	59.06	C
ATOM	4973	CG	PRO	C	169	53.155	106.932	197.426	1.00	62.55	C
ATOM	4974	C	PRO	C	169	50.956	109.720	196.509	1.00	60.12	C
ATOM	4975	O	PRO	C	169	51.072	110.473	197.471	1.00	61.83	C
ATOM	4976	N	MET	C	170	49.969	109.822	195.627	1.00	60.48	C
ATOM	4977	CA	MET	C	170	48.952	110.853	195.757	1.00	57.07	C
ATOM	4978	CB	MET	C	170	47.920	110.407	196.785	1.00	57.40	C
ATOM	4979	CG	MET	C	170	47.099	109.243	196.284	1.00	68.77	C
ATOM	4980	SD	MET	C	170	46.142	108.415	197.543	1.00	83.46	C
ATOM	4981	CE	MET	C	170	47.076	106.857	197.688	1.00	81.52	C
ATOM	4982	C	MET	C	170	49.586	112.177	196.155	1.00	55.70	C
ATOM	4983	O	MET	C	170	49.037	112.939	196.955	1.00	54.26	C
ATOM	4984	N	GLY	C	171	50.756	112.437	195.583	1.00	53.79	C
ATOM	4985	CA	GLY	C	171	51.467	113.661	195.872	1.00	57.23	C
ATOM	4986	C	GLY	C	171	52.107	114.207	194.617	1.00	62.42	C
ATOM	4987	O	GLY	C	171	51.736	113.817	193.510	1.00	65.08	C
ATOM	4988	N	GLU	C	172	53.076	115.101	194.780	1.00	65.84	C
ATOM	4989	CA	GLU	C	172	53.743	115.695	193.632	1.00	69.49	C
ATOM	4990	CB	GLU	C	172	52.823	116.742	193.001	1.00	74.68	C
ATOM	4991	CG	GLU	C	172	52.221	117.710	194.008	1.00	80.71	C
ATOM	4992	CD	GLU	C	172	51.095	118.526	193.414	1.00	86.58	C
ATOM	4993	OE1	GLU	C	172	51.365	119.305	192.475	1.00	87.16	C
ATOM	4994	OE2	GLU	C	172	49.940	118.383	193.879	1.00	90.77	C
ATOM	4995	C	GLU	C	172	55.092	116.317	193.971	1.00	68.52	C
ATOM	4996	O	GLU	C	172	55.402	116.574	195.128	1.00	67.20	C
ATOM	4997	N	SER	C	173	55.889	116.555	192.937	1.00	70.89	C



ATOM	4998	CA	SER	C	173	57.215	117.134	193.090	1.00	74.44	C
ATOM	4999	CB	SER	C	173	58.267	116.024	193.079	1.00	73.77	C
ATOM	5000	OG	SER	C	173	57.754	114.843	193.673	1.00	81.48	C
ATOM	5001	C	SER	C	173	57.469	118.076	191.920	1.00	76.32	C
ATOM	5002	O	SER	C	173	57.007	117.824	190.806	1.00	74.84	C
ATOM	5003	N	ALA	C	174	58.206	119.154	192.167	1.00	79.34	C
ATOM	5004	CA	ALA	C	174	58.508	120.101	191.104	1.00	81.62	C
ATOM	5005	CB	ALA	C	174	58.030	121.504	191.502	1.00	78.56	C
ATOM	5006	C	ALA	C	174	60.000	120.131	190.769	1.00	82.90	C
ATOM	5007	O	ALA	C	174	60.830	120.468	191.614	1.00	84.86	C
ATOM	5008	N	VAL	C	175	60.337	119.751	189.544	1.00	84.83	C
ATOM	5009	CA	VAL	C	175	61.719	119.783	189.091	1.00	90.74	C
ATOM	5010	CB	VAL	C	175	62.024	118.635	188.104	1.00	91.39	C
ATOM	5011	CG1	VAL	C	175	63.382	118.866	187.437	1.00	85.34	C
ATOM	5012	CG2	VAL	C	175	62.013	117.289	188.814	1.00	91.28	C
ATOM	5013	C	VAL	C	175	61.924	121.108	188.374	1.00	95.84	C
ATOM	5014	O	VAL	C	175	61.083	121.513	187.573	1.00	97.42	C
ATOM	5015	N	LYS	C	176	63.031	121.785	188.677	1.00	98.31	C
ATOM	5016	CA	LYS	C	176	63.317	123.077	188.060	1.00	101.27	C
ATOM	5017	CB	LYS	C	176	64.706	123.587	188.455	1.00	100.69	C
ATOM	5018	CG	LYS	C	176	64.846	123.986	189.934	1.00	103.93	C
ATOM	5019	CD	LYS	C	176	64.767	122.775	190.880	1.00	100.95	C
ATOM	5020	CE	LYS	C	176	65.184	123.136	192.311	1.00	93.35	C
ATOM	5021	NZ	LYS	C	176	64.327	124.214	192.885	1.00	85.34	C
ATOM	5022	C	LYS	C	176	63.239	122.973	186.534	1.00	105.72	C
ATOM	5023	O	LYS	C	176	64.022	122.258	185.906	1.00	105.99	C
ATOM	5024	N	LEU	C	177	62.280	123.688	185.947	1.00	109.01	C
ATOM	5025	CA	LEU	C	177	62.065	123.727	184.498	1.00	111.62	C
ATOM	5026	CB	LEU	C	177	60.600	124.081	184.244	1.00	108.02	C
ATOM	5027	CG	LEU	C	177	60.037	124.029	182.824	1.00	106.91	C
ATOM	5028	CD1	LEU	C	177	60.639	122.862	182.042	1.00	106.49	C
ATOM	5029	CD2	LEU	C	177	58.515	123.877	182.898	1.00	106.11	C
ATOM	5030	C	LEU	C	177	63.020	124.764	183.883	1.00	114.77	C
ATOM	5031	O	LEU	C	177	62.855	125.970	184.072	1.00	114.63	C
ATOM	5032	N	PRO	C	178	64.024	124.292	183.123	1.00	118.03	C
ATOM	5033	CD	PRO	C	178	64.136	122.874	182.734	1.00	118.62	C
ATOM	5034	CA	PRO	C	178	65.064	125.080	182.451	1.00	121.51	C
ATOM	5035	CB	PRO	C	178	65.963	124.004	181.858	1.00	119.90	C
ATOM	5036	CG	PRO	C	178	64.983	122.954	181.481	1.00	121.21	C
ATOM	5037	C	PRO	C	178	64.660	126.113	181.399	1.00	125.09	C
ATOM	5038	O	PRO	C	178	65.437	127.024	181.096	1.00	125.90	C
ATOM	5039	N	SER	C	179	63.463	125.973	180.837	1.00	127.68	C
ATOM	5040	CA	SER	C	179	62.962	126.883	179.799	1.00	129.15	C
ATOM	5041	CB	SER	C	179	63.203	128.352	180.184	1.00	130.38	C
ATOM	5042	OG	SER	C	179	62.503	129.226	179.311	1.00	132.50	C
ATOM	5043	C	SER	C	179	63.509	126.590	178.393	1.00	129.00	C
ATOM	5044	O	SER	C	179	62.984	127.098	177.389	1.00	128.49	C
ATOM	5045	N	ASP	C	180	64.574	125.787	178.331	1.00	128.89	C
ATOM	5046	CA	ASP	C	180	65.158	125.337	177.054	1.00	127.75	C
ATOM	5047	CB	ASP	C	180	66.561	124.741	177.273	1.00	128.01	C
ATOM	5048	CG	ASP	C	180	67.559	125.752	177.802	1.00	127.52	C
ATOM	5049	OD1	ASP	C	180	68.725	125.363	178.073	1.00	126.48	C
ATOM	5050	OD2	ASP	C	180	67.189	126.937	177.939	1.00	125.39	C
ATOM	5051	C	ASP	C	180	64.174	124.227	176.687	1.00	126.58	C
ATOM	5052	O	ASP	C	180	64.486	123.242	176.041	1.00	125.43	C
ATOM	5053	N	ALA	C	181	62.966	124.471	177.170	1.00	125.71	C
ATOM	5054	CA	ALA	C	181	61.768	123.655	177.100	1.00	124.62	C
ATOM	5055	CB	ALA	C	181	60.615	124.492	177.544	1.00	123.97	C



ATOM	5056	C	ALA	C	181	61.388	122.968	175.801	1.00124.67	C
ATOM	5057	O	ALA	C	181	62.219	122.587	174.974	1.00123.68	C
ATOM	5058	N	GLY	C	182	60.075	122.763	175.719	1.00125.40	C
ATOM	5059	CA	GLY	C	182	59.389	122.130	174.611	1.00126.58	C
ATOM	5060	C	GLY	C	182	57.968	121.923	175.103	1.00127.55	C
ATOM	5061	O	GLY	C	182	57.167	122.860	175.133	1.00129.15	C
ATOM	5062	N	SER	C	183	57.685	120.696	175.517	1.00126.04	C
ATOM	5063	CA	SER	C	183	56.393	120.289	176.035	1.00123.78	C
ATOM	5064	CB	SER	C	183	55.241	121.005	175.337	1.00124.79	C
ATOM	5065	OG	SER	C	183	54.093	121.012	176.171	1.00126.40	C
ATOM	5066	C	SER	C	183	56.384	118.825	175.675	1.00121.59	C
ATOM	5067	O	SER	C	183	55.507	118.058	176.075	1.00120.48	C
ATOM	5068	N	ASN	C	184	57.392	118.457	174.892	1.00119.90	C
ATOM	5069	CA	ASN	C	184	57.595	117.084	174.457	1.00118.04	C
ATOM	5070	CB	ASN	C	184	58.587	117.034	173.281	1.00117.77	C
ATOM	5071	CG	ASN	C	184	58.900	115.612	172.833	1.00117.70	C
ATOM	5072	OD1	ASN	C	184	58.005	114.873	172.418	1.00118.37	C
ATOM	5073	ND2	ASN	C	184	60.174	115.222	172.919	1.00117.12	C
ATOM	5074	C	ASN	C	184	58.179	116.366	175.661	1.00115.09	C
ATOM	5075	O	ASN	C	184	59.141	115.599	175.552	1.00114.37	C
ATOM	5076	N	ILE	C	185	57.603	116.652	176.823	1.00111.78	C
ATOM	5077	CA	ILE	C	185	58.061	116.041	178.057	1.00107.86	C
ATOM	5078	CB	ILE	C	185	57.105	116.358	179.225	1.00106.83	C
ATOM	5079	CG2	ILE	C	185	57.614	115.695	180.497	1.00107.60	C
ATOM	5080	CG1	ILE	C	185	57.014	117.874	179.429	1.00103.38	C
ATOM	5081	CD1	ILE	C	185	56.145	118.292	180.593	1.00100.79	C
ATOM	5082	C	ILE	C	185	58.173	114.526	177.876	1.00104.91	C
ATOM	5083	O	ILE	C	185	57.227	113.861	177.451	1.00104.46	C
ATOM	5084	N	THR	C	186	59.347	113.994	178.192	1.00 99.88	C
ATOM	5085	CA	THR	C	186	59.610	112.572	178.045	1.00 93.45	C
ATOM	5086	CB	THR	C	186	60.529	112.356	176.866	1.00 90.46	C
ATOM	5087	OG1	THR	C	186	61.627	113.268	176.956	1.00 91.77	C
ATOM	5088	CG2	THR	C	186	59.794	112.624	175.582	1.00 91.80	C
ATOM	5089	C	THR	C	186	60.237	111.972	179.298	1.00 89.73	C
ATOM	5090	O	THR	C	186	61.086	112.598	179.941	1.00 88.73	C
ATOM	5091	N	TYR	C	187	59.831	110.751	179.636	1.00 84.51	C
ATOM	5092	CA	TYR	C	187	60.343	110.119	180.843	1.00 76.69	C
ATOM	5093	CB	TYR	C	187	59.608	110.688	182.040	1.00 70.63	C
ATOM	5094	CG	TYR	C	187	58.169	110.248	182.070	1.00 65.83	C
ATOM	5095	CD1	TYR	C	187	57.813	108.990	182.552	1.00 67.66	C
ATOM	5096	CE1	TYR	C	187	56.496	108.564	182.554	1.00 64.58	C
ATOM	5097	CD2	TYR	C	187	57.166	111.071	181.588	1.00 66.42	C
ATOM	5098	CE2	TYR	C	187	55.842	110.656	181.584	1.00 66.81	C
ATOM	5099	CZ	TYR	C	187	55.515	109.402	182.069	1.00 66.60	C
ATOM	5100	OH	TYR	C	187	54.202	108.998	182.072	1.00 69.08	C
ATOM	5101	C	TYR	C	187	60.169	108.616	180.876	1.00 74.04	C
ATOM	5102	O	TYR	C	187	59.268	108.067	180.249	1.00 75.77	C
ATOM	5103	N	ARG	C	188	61.030	107.962	181.644	1.00 71.58	C
ATOM	5104	CA	ARG	C	188	60.966	106.519	181.852	1.00 66.93	C
ATOM	5105	CB	ARG	C	188	62.210	105.844	181.279	1.00 66.96	C
ATOM	5106	CG	ARG	C	188	62.498	106.217	179.832	1.00 73.84	C
ATOM	5107	CD	ARG	C	188	63.851	105.699	179.371	1.00 76.28	C
ATOM	5108	NE	ARG	C	188	63.885	104.246	179.258	1.00 83.41	C
ATOM	5109	CZ	ARG	C	188	63.207	103.555	178.347	1.00 86.78	C
ATOM	5110	NH1	ARG	C	188	62.442	104.189	177.469	1.00 86.61	C
ATOM	5111	NH2	ARG	C	188	63.294	102.230	178.310	1.00 89.02	C
ATOM	5112	C	ARG	C	188	60.966	106.425	183.380	1.00 63.56	C
ATOM	5113	O	ARG	C	188	61.206	107.431	184.054	1.00 66.39	C



ATOM	5114	N	THR	C	189	60.666	105.265	183.948	1.00	56.26	C
ATOM	5115	CA	THR	C	189	60.709	105.175	185.406	1.00	51.73	C
ATOM	5116	CB	THR	C	189	59.328	105.165	186.053	1.00	44.57	C
ATOM	5117	OG1	THR	C	189	58.750	103.867	185.906	1.00	40.53	C
ATOM	5118	CG2	THR	C	189	58.444	106.219	185.435	1.00	44.58	C
ATOM	5119	C	THR	C	189	61.431	103.921	185.850	1.00	52.18	C
ATOM	5120	O	THR	C	189	61.963	103.178	185.023	1.00	54.16	C
ATOM	5121	N	ILE	C	190	61.461	103.687	187.159	1.00	48.53	C
ATOM	5122	CA	ILE	C	190	62.142	102.517	187.674	1.00	42.95	C
ATOM	5123	CB	ILE	C	190	63.328	102.952	188.545	1.00	37.82	C
ATOM	5124	CG2	ILE	C	190	64.168	101.754	188.935	1.00	36.28	C
ATOM	5125	CG1	ILE	C	190	64.180	103.942	187.738	1.00	37.12	C
ATOM	5126	CD1	ILE	C	190	65.488	104.346	188.358	1.00	25.84	C
ATOM	5127	C	ILE	C	190	61.155	101.635	188.424	1.00	44.75	C
ATOM	5128	O	ILE	C	190	60.578	102.032	189.439	1.00	48.31	C
ATOM	5129	N	ASN	C	191	60.947	100.433	187.897	1.00	42.33	C
ATOM	5130	CA	ASN	C	191	60.003	99.496	188.490	1.00	40.95	C
ATOM	5131	CB	ASN	C	191	59.467	98.550	187.426	1.00	42.10	C
ATOM	5132	CG	ASN	C	191	60.565	97.712	186.800	1.00	44.85	C
ATOM	5133	OD1	ASN	C	191	61.391	97.099	187.491	1.00	46.32	C
ATOM	5134	ND2	ASN	C	191	60.578	97.678	185.485	1.00	45.05	C
ATOM	5135	C	ASN	C	191	60.592	98.653	189.605	1.00	37.68	C
ATOM	5136	O	ASN	C	191	61.810	98.641	189.834	1.00	36.56	C
ATOM	5137	N	ASP	C	192	59.687	97.925	190.252	1.00	29.54	C
ATOM	5138	CA	ASP	C	192	59.980	97.038	191.355	1.00	26.12	C
ATOM	5139	CB	ASP	C	192	58.794	96.105	191.590	1.00	29.81	C
ATOM	5140	CG	ASP	C	192	57.530	96.835	192.038	1.00	37.12	C
ATOM	5141	OD1	ASP	C	192	56.574	96.135	192.421	1.00	38.10	C
ATOM	5142	OD2	ASP	C	192	57.482	98.084	192.017	1.00	41.01	C
ATOM	5143	C	ASP	C	192	61.221	96.184	191.158	1.00	30.47	C
ATOM	5144	O	ASP	C	192	61.752	95.623	192.115	1.00	31.14	C
ATOM	5145	N	TYR	C	193	61.698	96.069	189.926	1.00	34.05	C
ATOM	5146	CA	TYR	C	193	62.862	95.228	189.682	1.00	37.89	C
ATOM	5147	CB	TYR	C	193	62.568	94.254	188.547	1.00	39.92	C
ATOM	5148	CG	TYR	C	193	61.238	93.590	188.748	1.00	42.75	C
ATOM	5149	CD1	TYR	C	193	60.125	93.989	188.016	1.00	43.39	C
ATOM	5150	CE1	TYR	C	193	58.869	93.439	188.264	1.00	49.48	C
ATOM	5151	CD2	TYR	C	193	61.069	92.619	189.738	1.00	45.79	C
ATOM	5152	CE2	TYR	C	193	59.820	92.062	189.997	1.00	48.41	C
ATOM	5153	CZ	TYR	C	193	58.723	92.475	189.255	1.00	48.31	C
ATOM	5154	OH	TYR	C	193	57.484	91.926	189.495	1.00	48.52	C
ATOM	5155	C	TYR	C	193	64.059	96.066	189.369	1.00	39.57	C
ATOM	5156	O	TYR	C	193	65.084	95.565	188.902	1.00	39.00	C
ATOM	5157	N	GLY	C	194	63.919	97.354	189.649	1.00	42.47	C
ATOM	5158	CA	GLY	C	194	65.006	98.275	189.411	1.00	46.94	C
ATOM	5159	C	GLY	C	194	65.286	98.314	187.938	1.00	46.53	C
ATOM	5160	O	GLY	C	194	66.421	98.531	187.511	1.00	42.21	C
ATOM	5161	N	ALA	C	195	64.224	98.093	187.170	1.00	50.72	C
ATOM	5162	CA	ALA	C	195	64.296	98.082	185.720	1.00	53.38	C
ATOM	5163	CB	ALA	C	195	63.659	96.797	185.193	1.00	56.76	C
ATOM	5164	C	ALA	C	195	63.592	99.315	185.140	1.00	53.03	C
ATOM	5165	O	ALA	C	195	62.570	99.761	185.670	1.00	45.75	C
ATOM	5166	N	LEU	C	196	64.162	99.860	184.065	1.00	57.23	C
ATOM	5167	CA	LEU	C	196	63.613	101.036	183.396	1.00	61.31	C
ATOM	5168	CB	LEU	C	196	64.627	101.616	182.406	1.00	61.57	C
ATOM	5169	CG	LEU	C	196	65.827	102.392	182.958	1.00	66.94	C
ATOM	5170	CD1	LEU	C	196	66.805	102.733	181.837	1.00	63.88	C
ATOM	5171	CD2	LEU	C	196	65.333	103.655	183.638	1.00	63.34	C



ATOM	5172	C	LEU	C	196	62.354	100.679	182.635	1.00	64.83	C
ATOM	5173	O	LEU	C	196	62.350	99.756	181.827	1.00	70.03	C
ATOM	5174	N	THR	C	197	61.275	101.400	182.894	1.00	66.18	C
ATOM	5175	CA	THR	C	197	60.047	101.125	182.181	1.00	66.57	C
ATOM	5176	CB	THR	C	197	58.826	101.751	182.880	1.00	65.48	C
ATOM	5177	OG1	THR	C	197	58.916	103.182	182.833	1.00	63.03	C
ATOM	5178	CG2	THR	C	197	58.760	101.278	184.324	1.00	63.15	C
ATOM	5179	C	THR	C	197	60.242	101.747	180.807	1.00	69.53	C
ATOM	5180	O	THR	C	197	61.224	102.457	180.575	1.00	67.83	C
ATOM	5181	N	PRO	C	198	59.325	101.477	179.869	1.00	72.51	C
ATOM	5182	CD	PRO	C	198	58.157	100.578	179.920	1.00	71.55	C
ATOM	5183	CA	PRO	C	198	59.480	102.058	178.535	1.00	74.44	C
ATOM	5184	CB	PRO	C	198	58.509	101.235	177.696	1.00	73.13	C
ATOM	5185	CG	PRO	C	198	57.404	100.955	178.670	1.00	71.33	C
ATOM	5186	C	PRO	C	198	59.164	103.554	178.511	1.00	75.99	C
ATOM	5187	O	PRO	C	198	58.261	104.026	179.216	1.00	75.66	C
ATOM	5188	N	LYS	C	199	59.924	104.284	177.696	1.00	76.63	C
ATOM	5189	CA	LYS	C	199	59.772	105.730	177.528	1.00	75.31	C
ATOM	5190	CB	LYS	C	199	60.701	106.193	176.408	1.00	73.36	C
ATOM	5191	CG	LYS	C	199	60.569	107.635	175.978	1.00	78.70	C
ATOM	5192	CD	LYS	C	199	61.732	107.963	175.029	1.00	84.97	C
ATOM	5193	CE	LYS	C	199	61.457	109.156	174.109	1.00	87.72	C
ATOM	5194	NZ	LYS	C	199	61.303	110.446	174.828	1.00	84.39	C
ATOM	5195	C	LYS	C	199	58.332	106.110	177.212	1.00	74.66	C
ATOM	5196	O	LYS	C	199	57.708	105.522	176.338	1.00	76.81	C
ATOM	5197	N	MET	C	200	57.793	107.081	177.936	1.00	75.62	C
ATOM	5198	CA	MET	C	200	56.423	107.512	177.698	1.00	76.90	C
ATOM	5199	CB	MET	C	200	55.531	107.175	178.887	1.00	79.40	C
ATOM	5200	CG	MET	C	200	56.138	106.183	179.849	1.00	84.53	C
ATOM	5201	SD	MET	C	200	54.880	105.376	180.856	1.00	94.91	C
ATOM	5202	CE	MET	C	200	55.414	103.653	180.693	1.00	91.76	C
ATOM	5203	C	MET	C	200	56.432	109.011	177.476	1.00	76.45	C
ATOM	5204	O	MET	C	200	57.414	109.679	177.808	1.00	75.14	C
ATOM	5205	N	THR	C	201	55.340	109.536	176.923	1.00	76.88	C
ATOM	5206	CA	THR	C	201	55.242	110.966	176.637	1.00	77.61	C
ATOM	5207	CB	THR	C	201	54.532	111.218	175.282	1.00	76.28	C
ATOM	5208	OG1	THR	C	201	55.271	110.584	174.228	1.00	74.52	C
ATOM	5209	CG2	THR	C	201	54.446	112.715	174.998	1.00	73.93	C
ATOM	5210	C	THR	C	201	54.532	111.782	177.709	1.00	76.90	C
ATOM	5211	O	THR	C	201	53.459	111.410	178.187	1.00	76.37	C
ATOM	5212	N	GLY	C	202	55.145	112.904	178.067	1.00	77.52	C
ATOM	5213	CA	GLY	C	202	54.575	113.784	179.066	1.00	81.83	C
ATOM	5214	C	GLY	C	202	53.168	114.189	178.687	1.00	85.10	C
ATOM	5215	O	GLY	C	202	52.908	114.537	177.535	1.00	85.51	C
ATOM	5216	N	VAL	C	203	52.263	114.147	179.660	1.00	87.70	C
ATOM	5217	CA	VAL	C	203	50.863	114.490	179.435	1.00	89.74	C
ATOM	5218	CB	VAL	C	203	49.993	113.223	179.513	1.00	88.84	C
ATOM	5219	CG1	VAL	C	203	48.551	113.548	179.167	1.00	85.33	C
ATOM	5220	CG2	VAL	C	203	50.555	112.161	178.587	1.00	85.34	C
ATOM	5221	C	VAL	C	203	50.364	115.497	180.468	1.00	93.55	C
ATOM	5222	O	VAL	C	203	49.618	115.138	181.383	1.00	96.77	C
ATOM	5223	N	MET	C	204	50.772	116.755	180.314	1.00	95.77	C
ATOM	5224	CA	MET	C	204	50.388	117.826	181.242	1.00	98.27	C
ATOM	5225	CB	MET	C	204	50.684	119.198	180.621	1.00	100.85	C
ATOM	5226	CG	MET	C	204	52.162	119.467	180.325	1.00	106.92	C
ATOM	5227	SD	MET	C	204	52.917	118.333	179.108	1.00	114.76	C
ATOM	5228	CE	MET	C	204	52.536	119.164	177.564	1.00	110.79	C
ATOM	5229	C	MET	C	204	48.920	117.763	181.658	1.00	97.63	C



ATOM	5230	O	MET	C	204	48.040	117.606	180.822	1.00	96.53	C
ATOM	5231	N	GLU	C	205	48.662	117.880	182.956	1.00	99.36	C
ATOM	5232	CA	GLU	C	205	47.295	117.841	183.458	1.00	102.30	C
ATOM	5233	CB	GLU	C	205	47.241	117.308	184.894	1.00	106.56	C
ATOM	5234	CG	GLU	C	205	47.761	118.284	185.952	1.00	114.04	C
ATOM	5235	CD	GLU	C	205	46.764	118.527	187.085	1.00	117.38	C
ATOM	5236	OE1	GLU	C	205	47.091	119.296	188.021	1.00	117.73	C
ATOM	5237	OE2	GLU	C	205	45.656	117.949	187.037	1.00	117.98	C
ATOM	5238	C	GLU	C	205	46.735	119.251	183.430	1.00	102.90	C
ATOM	5239	O	GLU	C	205	45.552	119.399	183.065	1.00	102.02	C
ATOM	5240	OXT	GLU	C	205	47.488	120.185	183.792	1.00	104.63	C
ATOM	5241	CB	PHE	D	1	57.259	55.852	168.279	1.00	36.89	D
ATOM	5242	CG	PHE	D	1	57.904	56.830	169.212	1.00	36.42	D
ATOM	5243	CD1	PHE	D	1	58.083	58.162	168.840	1.00	38.81	D
ATOM	5244	CD2	PHE	D	1	58.291	56.437	170.485	1.00	39.03	D
ATOM	5245	CE1	PHE	D	1	58.630	59.083	169.723	1.00	30.53	D
ATOM	5246	CE2	PHE	D	1	58.844	57.353	171.383	1.00	31.99	D
ATOM	5247	CZ	PHE	D	1	59.011	58.680	170.996	1.00	35.83	D
ATOM	5248	C	PHE	D	1	55.160	57.227	168.009	1.00	32.04	D
ATOM	5249	O	PHE	D	1	55.302	57.704	166.893	1.00	29.74	D
ATOM	5250	N	PHE	D	1	55.170	54.904	167.334	1.00	41.01	D
ATOM	5251	CA	PHE	D	1	55.720	55.855	168.338	1.00	36.16	D
ATOM	5252	N	ALA	D	2	54.499	57.841	168.983	1.00	32.31	D
ATOM	5253	CA	ALA	D	2	53.909	59.163	168.807	1.00	29.54	D
ATOM	5254	CB	ALA	D	2	52.482	59.024	168.380	1.00	22.02	D
ATOM	5255	C	ALA	D	2	53.988	59.937	170.119	1.00	29.62	D
ATOM	5256	O	ALA	D	2	54.118	59.341	171.191	1.00	30.32	D
ATOM	5257	N	CYS	D	3	53.903	61.259	170.044	1.00	25.22	D
ATOM	5258	CA	CYS	D	3	53.978	62.063	171.250	1.00	25.37	D
ATOM	5259	C	CYS	D	3	52.871	63.107	171.263	1.00	26.10	D
ATOM	5260	O	CYS	D	3	52.303	63.424	170.233	1.00	28.50	D
ATOM	5261	CB	CYS	D	3	55.330	62.762	171.333	1.00	29.28	D
ATOM	5262	SG	CYS	D	3	56.828	61.724	171.199	1.00	39.44	D
ATOM	5263	N	LYS	D	4	52.553	63.634	172.437	1.00	29.28	D
ATOM	5264	CA	LYS	D	4	51.523	64.653	172.548	1.00	33.89	D
ATOM	5265	CB	LYS	D	4	50.165	64.057	172.936	1.00	32.29	D
ATOM	5266	CG	LYS	D	4	50.124	63.470	174.338	1.00	45.50	D
ATOM	5267	CD	LYS	D	4	48.805	62.752	174.661	1.00	51.16	D
ATOM	5268	CE	LYS	D	4	47.638	63.710	174.816	1.00	56.15	D
ATOM	5269	NZ	LYS	D	4	47.300	64.394	173.535	1.00	65.92	D
ATOM	5270	C	LYS	D	4	51.930	65.680	173.586	1.00	37.28	D
ATOM	5271	O	LYS	D	4	52.777	65.448	174.448	1.00	35.47	D
ATOM	5272	N	THR	D	5	51.284	66.825	173.487	1.00	40.33	D
ATOM	5273	CA	THR	D	5	51.549	67.934	174.357	1.00	37.06	D
ATOM	5274	CB	THR	D	5	51.693	69.212	173.492	1.00	33.03	D
ATOM	5275	OG1	THR	D	5	52.879	69.904	173.879	1.00	37.46	D
ATOM	5276	CG2	THR	D	5	50.502	70.096	173.596	1.00	22.34	D
ATOM	5277	C	THR	D	5	50.430	68.013	175.377	1.00	36.30	D
ATOM	5278	O	THR	D	5	49.260	67.825	175.053	1.00	38.39	D
ATOM	5279	N	ALA	D	6	50.809	68.252	176.624	1.00	35.55	D
ATOM	5280	CA	ALA	D	6	49.860	68.345	177.719	1.00	34.84	D
ATOM	5281	CB	ALA	D	6	50.579	68.735	178.996	1.00	35.68	D
ATOM	5282	C	ALA	D	6	48.779	69.345	177.410	1.00	38.31	D
ATOM	5283	O	ALA	D	6	47.663	69.249	177.911	1.00	41.55	D
ATOM	5284	N	ASN	D	7	49.115	70.312	176.571	1.00	44.27	D
ATOM	5285	CA	ASN	D	7	48.174	71.352	176.191	1.00	48.59	D
ATOM	5286	CB	ASN	D	7	48.912	72.486	175.502	1.00	51.23	D
ATOM	5287	CG	ASN	D	7	48.371	73.830	175.881	1.00	57.00	D



ATOM	5288	OD1	ASN	D	7	47.359	73.923	176.586	1.00	61.41	D
ATOM	5289	ND2	ASN	D	7	49.034	74.890	175.419	1.00	45.59	D
ATOM	5290	C	ASN	D	7	47.120	70.800	175.260	1.00	49.26	D
ATOM	5291	O	ASN	D	7	45.948	71.185	175.327	1.00	54.86	D
ATOM	5292	N	GLY	D	8	47.558	69.903	174.388	1.00	47.30	D
ATOM	5293	CA	GLY	D	8	46.659	69.282	173.446	1.00	52.30	D
ATOM	5294	C	GLY	D	8	47.332	68.681	172.216	1.00	57.17	D
ATOM	5295	O	GLY	D	8	47.081	67.509	171.881	1.00	59.28	D
ATOM	5296	N	THR	D	9	48.191	69.466	171.555	1.00	52.59	D
ATOM	5297	CA	THR	D	9	48.865	69.061	170.318	1.00	47.80	D
ATOM	5298	CB	THR	D	9	49.710	70.196	169.811	1.00	49.09	D
ATOM	5299	OG1	THR	D	9	48.871	71.346	169.659	1.00	59.62	D
ATOM	5300	CG2	THR	D	9	50.327	69.849	168.468	1.00	51.33	D
ATOM	5301	C	THR	D	9	49.694	67.780	170.266	1.00	46.47	D
ATOM	5302	O	THR	D	9	50.365	67.414	171.223	1.00	47.30	D
ATOM	5303	N	ALA	D	10	49.644	67.114	169.110	1.00	43.63	D
ATOM	5304	CA	ALA	D	10	50.347	65.854	168.881	1.00	38.68	D
ATOM	5305	CB	ALA	D	10	49.343	64.721	168.749	1.00	28.38	D
ATOM	5306	C	ALA	D	10	51.215	65.856	167.650	1.00	38.13	D
ATOM	5307	O	ALA	D	10	51.013	66.650	166.731	1.00	42.10	D
ATOM	5308	N	ILE	D	11	52.193	64.961	167.647	1.00	35.07	D
ATOM	5309	CA	ILE	D	11	53.061	64.782	166.501	1.00	33.71	D
ATOM	5310	CB	ILE	D	11	54.501	65.081	166.810	1.00	33.38	D
ATOM	5311	CG2	ILE	D	11	55.324	64.872	165.545	1.00	34.59	D
ATOM	5312	CG1	ILE	D	11	54.633	66.517	167.333	1.00	34.65	D
ATOM	5313	CD1	ILE	D	11	56.046	66.919	167.709	1.00	36.71	D
ATOM	5314	C	ILE	D	11	52.898	63.300	166.268	1.00	34.43	D
ATOM	5315	O	ILE	D	11	53.236	62.497	167.123	1.00	40.94	D
ATOM	5316	N	PRO	D	12	52.372	62.914	165.108	1.00	31.48	D
ATOM	5317	CD	PRO	D	12	51.959	63.780	163.988	1.00	35.92	D
ATOM	5318	CA	PRO	D	12	52.147	61.507	164.782	1.00	31.33	D
ATOM	5319	CB	PRO	D	12	51.135	61.592	163.651	1.00	35.15	D
ATOM	5320	CG	PRO	D	12	51.669	62.771	162.868	1.00	36.13	D
ATOM	5321	C	PRO	D	12	53.348	60.680	164.385	1.00	31.60	D
ATOM	5322	O	PRO	D	12	54.466	61.192	164.304	1.00	29.52	D
ATOM	5323	N	ILE	D	13	53.069	59.393	164.141	1.00	31.67	D
ATOM	5324	CA	ILE	D	13	54.040	58.388	163.700	1.00	31.87	D
ATOM	5325	CB	ILE	D	13	53.314	57.085	163.279	1.00	32.42	D
ATOM	5326	CG2	ILE	D	13	54.258	56.158	162.495	1.00	34.06	D
ATOM	5327	CG1	ILE	D	13	52.741	56.393	164.517	1.00	27.64	D
ATOM	5328	CD1	ILE	D	13	51.986	55.157	164.210	1.00	23.75	D
ATOM	5329	C	ILE	D	13	54.753	58.953	162.483	1.00	33.11	D
ATOM	5330	O	ILE	D	13	54.092	59.437	161.571	1.00	36.32	D
ATOM	5331	N	GLY	D	14	56.084	58.899	162.466	1.00	30.35	D
ATOM	5332	CA	GLY	D	14	56.827	59.432	161.337	1.00	30.86	D
ATOM	5333	C	GLY	D	14	57.452	60.788	161.631	1.00	35.11	D
ATOM	5334	O	GLY	D	14	58.229	61.325	160.832	1.00	37.52	D
ATOM	5335	N	GLY	D	15	57.096	61.362	162.775	1.00	34.23	D
ATOM	5336	CA	GLY	D	15	57.662	62.642	163.161	1.00	31.45	D
ATOM	5337	C	GLY	D	15	56.914	63.872	162.695	1.00	32.59	D
ATOM	5338	O	GLY	D	15	55.895	63.782	162.014	1.00	36.23	D
ATOM	5339	N	GLY	D	16	57.443	65.035	163.064	1.00	30.04	D
ATOM	5340	CA	GLY	D	16	56.828	66.300	162.715	1.00	21.60	D
ATOM	5341	C	GLY	D	16	57.194	67.311	163.780	1.00	20.80	D
ATOM	5342	O	GLY	D	16	58.195	67.152	164.467	1.00	23.81	D
ATOM	5343	N	SER	D	17	56.385	68.336	163.973	1.00	17.38	D
ATOM	5344	CA	SER	D	17	56.755	69.317	164.968	1.00	15.97	D
ATOM	5345	CB	SER	D	17	57.572	70.425	164.303	1.00	22.87	D



ATOM	5346	OG	SER	D	17	56.748	71.269	163.514	1.00	30.46	D
ATOM	5347	C	SER	D	17	55.581	69.927	165.691	1.00	14.56	D
ATOM	5348	O	SER	D	17	54.463	69.931	165.177	1.00	14.95	D
ATOM	5349	N	ALA	D	18	55.830	70.452	166.888	1.00	13.49	D
ATOM	5350	CA	ALA	D	18	54.764	71.078	167.657	1.00	14.66	D
ATOM	5351	CB	ALA	D	18	54.017	70.041	168.466	1.00	13.05	D
ATOM	5352	C	ALA	D	18	55.284	72.144	168.579	1.00	22.81	D
ATOM	5353	O	ALA	D	18	56.458	72.149	168.960	1.00	29.79	D
ATOM	5354	N	ASN	D	19	54.383	73.049	168.939	1.00	23.69	D
ATOM	5355	CA	ASN	D	19	54.685	74.139	169.842	1.00	20.68	D
ATOM	5356	CB	ASN	D	19	53.772	75.334	169.562	1.00	17.54	D
ATOM	5357	CG	ASN	D	19	54.211	76.135	168.361	1.00	16.26	D
ATOM	5358	OD1	ASN	D	19	55.198	75.797	167.706	1.00	13.52	D
ATOM	5359	ND2	ASN	D	19	53.479	77.211	168.061	1.00	6.31	D
ATOM	5360	C	ASN	D	19	54.433	73.692	171.260	1.00	22.94	D
ATOM	5361	O	ASN	D	19	53.491	72.961	171.532	1.00	25.61	D
ATOM	5362	N	VAL	D	20	55.268	74.139	172.177	1.00	26.10	D
ATOM	5363	CA	VAL	D	20	55.046	73.808	173.569	1.00	29.01	D
ATOM	5364	CB	VAL	D	20	56.117	72.866	174.082	1.00	30.34	D
ATOM	5365	CG1	VAL	D	20	55.786	72.461	175.499	1.00	36.31	D
ATOM	5366	CG2	VAL	D	20	56.179	71.651	173.185	1.00	17.55	D
ATOM	5367	C	VAL	D	20	55.078	75.128	174.330	1.00	27.78	D
ATOM	5368	O	VAL	D	20	56.125	75.754	174.430	1.00	28.94	D
ATOM	5369	N	TYR	D	21	53.926	75.543	174.846	1.00	26.42	D
ATOM	5370	CA	TYR	D	21	53.794	76.808	175.578	1.00	28.63	D
ATOM	5371	CB	TYR	D	21	52.419	77.409	175.286	1.00	22.74	D
ATOM	5372	CG	TYR	D	21	52.116	77.456	173.815	1.00	27.07	D
ATOM	5373	CD1	TYR	D	21	51.297	76.508	173.226	1.00	24.22	D
ATOM	5374	CE1	TYR	D	21	51.046	76.526	171.850	1.00	29.42	D
ATOM	5375	CD2	TYR	D	21	52.687	78.439	172.994	1.00	30.98	D
ATOM	5376	CE2	TYR	D	21	52.445	78.471	171.627	1.00	29.68	D
ATOM	5377	CZ	TYR	D	21	51.620	77.510	171.060	1.00	35.48	D
ATOM	5378	OH	TYR	D	21	51.339	77.546	169.714	1.00	35.61	D
ATOM	5379	C	TYR	D	21	53.999	76.690	177.096	1.00	31.93	D
ATOM	5380	O	TYR	D	21	53.221	76.019	177.792	1.00	34.89	D
ATOM	5381	N	VAL	D	22	55.020	77.377	177.610	1.00	31.86	D
ATOM	5382	CA	VAL	D	22	55.355	77.318	179.042	1.00	31.50	D
ATOM	5383	CB	VAL	D	22	56.776	76.822	179.262	1.00	29.55	D
ATOM	5384	CG1	VAL	D	22	56.952	75.463	178.647	1.00	27.42	D
ATOM	5385	CG2	VAL	D	22	57.745	77.823	178.690	1.00	25.10	D
ATOM	5386	C	VAL	D	22	55.282	78.593	179.859	1.00	30.58	D
ATOM	5387	O	VAL	D	22	55.792	79.628	179.434	1.00	31.73	D
ATOM	5388	N	ASN	D	23	54.678	78.498	181.045	1.00	30.13	D
ATOM	5389	CA	ASN	D	23	54.608	79.633	181.965	1.00	33.35	D
ATOM	5390	CB	ASN	D	23	53.389	79.516	182.841	1.00	34.26	D
ATOM	5391	CG	ASN	D	23	52.179	79.108	182.073	1.00	33.36	D
ATOM	5392	OD1	ASN	D	23	51.426	79.934	181.556	1.00	31.84	D
ATOM	5393	ND2	ASN	D	23	51.988	77.811	181.970	1.00	45.18	D
ATOM	5394	C	ASN	D	23	55.863	79.499	182.836	1.00	35.03	D
ATOM	5395	O	ASN	D	23	56.071	78.456	183.453	1.00	31.46	D
ATOM	5396	N	LEU	D	24	56.698	80.538	182.872	1.00	35.88	D
ATOM	5397	CA	LEU	D	24	57.942	80.505	183.645	1.00	35.56	D
ATOM	5398	CB	LEU	D	24	59.100	80.956	182.758	1.00	31.96	D
ATOM	5399	CG	LEU	D	24	59.274	80.276	181.399	1.00	26.28	D
ATOM	5400	CD1	LEU	D	24	59.974	81.234	180.457	1.00	18.62	D
ATOM	5401	CD2	LEU	D	24	60.070	78.992	181.523	1.00	26.70	D
ATOM	5402	C	LEU	D	24	57.908	81.399	184.888	1.00	35.50	D
ATOM	5403	O	LEU	D	24	57.108	82.331	184.965	1.00	38.67	D



ATOM	5404	N	ALA	D	25	58.771	81.106	185.861	1.00	33.58	D
ATOM	5405	CA	ALA	D	25	58.875	81.923	187.080	1.00	31.95	D
ATOM	5406	CB	ALA	D	25	60.106	81.539	187.835	1.00	24.42	D
ATOM	5407	C	ALA	D	25	59.000	83.369	186.607	1.00	33.36	D
ATOM	5408	O	ALA	D	25	59.872	83.691	185.812	1.00	39.23	D
ATOM	5409	N	PRO	D	26	58.149	84.261	187.095	1.00	29.18	D
ATOM	5410	CD	PRO	D	26	57.140	84.050	188.131	1.00	31.01	D
ATOM	5411	CA	PRO	D	26	58.188	85.672	186.682	1.00	33.36	D
ATOM	5412	CB	PRO	D	26	56.976	86.288	187.406	1.00	34.37	D
ATOM	5413	CG	PRO	D	26	56.133	85.132	187.779	1.00	41.30	D
ATOM	5414	C	PRO	D	26	59.476	86.466	186.991	1.00	35.68	D
ATOM	5415	O	PRO	D	26	59.792	87.443	186.300	1.00	33.16	D
ATOM	5416	N	VAL	D	27	60.184	86.046	188.040	1.00	34.83	D
ATOM	5417	CA	VAL	D	27	61.402	86.687	188.502	1.00	32.24	D
ATOM	5418	CB	VAL	D	27	61.137	87.469	189.780	1.00	34.79	D
ATOM	5419	CG1	VAL	D	27	62.437	88.011	190.338	1.00	34.21	D
ATOM	5420	CG2	VAL	D	27	60.143	88.574	189.507	1.00	34.74	D
ATOM	5421	C	VAL	D	27	62.486	85.683	188.831	1.00	33.29	D
ATOM	5422	O	VAL	D	27	62.237	84.684	189.495	1.00	36.62	D
ATOM	5423	N	VAL	D	28	63.700	85.965	188.389	1.00	33.27	D
ATOM	5424	CA	VAL	D	28	64.824	85.087	188.660	1.00	35.23	D
ATOM	5425	CB	VAL	D	28	65.087	84.146	187.461	1.00	33.34	D
ATOM	5426	CG1	VAL	D	28	66.202	83.151	187.786	1.00	35.25	D
ATOM	5427	CG2	VAL	D	28	63.808	83.420	187.097	1.00	31.50	D
ATOM	5428	C	VAL	D	28	66.021	86.012	188.883	1.00	40.85	D
ATOM	5429	O	VAL	D	28	66.215	86.994	188.154	1.00	44.35	D
ATOM	5430	N	ASN	D	29	66.826	85.710	189.895	1.00	40.68	D
ATOM	5431	CA	ASN	D	29	67.975	86.552	190.191	1.00	37.56	D
ATOM	5432	CB	ASN	D	29	68.204	86.652	191.694	1.00	30.21	D
ATOM	5433	CG	ASN	D	29	67.004	87.167	192.423	1.00	33.80	D
ATOM	5434	OD1	ASN	D	29	66.495	88.237	192.117	1.00	35.33	D
ATOM	5435	ND2	ASN	D	29	66.536	86.405	193.406	1.00	43.52	D
ATOM	5436	C	ASN	D	29	69.227	86.010	189.575	1.00	36.11	D
ATOM	5437	O	ASN	D	29	69.333	84.810	189.306	1.00	31.46	D
ATOM	5438	N	VAL	D	30	70.183	86.906	189.368	1.00	34.45	D
ATOM	5439	CA	VAL	D	30	71.461	86.497	188.835	1.00	35.36	D
ATOM	5440	CB	VAL	D	30	72.463	87.664	188.859	1.00	32.27	D
ATOM	5441	CG1	VAL	D	30	73.841	87.190	188.390	1.00	29.74	D
ATOM	5442	CG2	VAL	D	30	71.954	88.797	187.968	1.00	27.96	D
ATOM	5443	C	VAL	D	30	71.900	85.414	189.811	1.00	39.31	D
ATOM	5444	O	VAL	D	30	71.595	85.498	191.002	1.00	36.78	D
ATOM	5445	N	GLY	D	31	72.576	84.387	189.309	1.00	44.19	D
ATOM	5446	CA	GLY	D	31	73.031	83.321	190.185	1.00	48.84	D
ATOM	5447	C	GLY	D	31	72.044	82.180	190.375	1.00	50.83	D
ATOM	5448	O	GLY	D	31	72.464	81.044	190.574	1.00	52.00	D
ATOM	5449	N	GLN	D	32	70.744	82.466	190.316	1.00	49.73	D
ATOM	5450	CA	GLN	D	32	69.724	81.433	190.485	1.00	50.93	D
ATOM	5451	CB	GLN	D	32	68.430	82.067	190.983	1.00	52.59	D
ATOM	5452	CG	GLN	D	32	68.335	82.166	192.489	1.00	62.57	D
ATOM	5453	CD	GLN	D	32	67.252	83.134	192.937	1.00	67.08	D
ATOM	5454	OE1	GLN	D	32	66.156	83.172	192.363	1.00	66.36	D
ATOM	5455	NE2	GLN	D	32	67.551	83.917	193.978	1.00	68.68	D
ATOM	5456	C	GLN	D	32	69.431	80.603	189.220	1.00	52.33	D
ATOM	5457	O	GLN	D	32	70.000	80.829	188.148	1.00	51.38	D
ATOM	5458	N	ASN	D	33	68.544	79.625	189.368	1.00	49.70	D
ATOM	5459	CA	ASN	D	33	68.155	78.758	188.266	1.00	47.04	D
ATOM	5460	CB	ASN	D	33	68.312	77.293	188.656	1.00	40.13	D
ATOM	5461	CG	ASN	D	33	69.625	76.705	188.208	1.00	46.47	D



ATOM	5462	OD1	ASN	D	33	69.998	75.601	188.623	1.00	39.03	D
ATOM	5463	ND2	ASN	D	33	70.335	77.424	187.344	1.00	45.09	D
ATOM	5464	C	ASN	D	33	66.714	78.961	187.819	1.00	50.10	D
ATOM	5465	O	ASN	D	33	65.782	79.029	188.624	1.00	52.06	D
ATOM	5466	N	LEU	D	34	66.536	79.084	186.518	1.00	51.65	D
ATOM	5467	CA	LEU	D	34	65.205	79.188	185.957	1.00	50.51	D
ATOM	5468	CB	LEU	D	34	65.180	80.156	184.787	1.00	47.71	D
ATOM	5469	CG	LEU	D	34	63.904	80.080	183.962	1.00	43.39	D
ATOM	5470	CD1	LEU	D	34	62.755	80.760	184.687	1.00	37.93	D
ATOM	5471	CD2	LEU	D	34	64.171	80.738	182.622	1.00	47.60	D
ATOM	5472	C	LEU	D	34	65.042	77.753	185.453	1.00	50.83	D
ATOM	5473	O	LEU	D	34	65.919	77.218	184.748	1.00	47.19	D
ATOM	5474	N	VAL	D	35	63.949	77.113	185.830	1.00	47.27	D
ATOM	5475	CA	VAL	D	35	63.773	75.744	185.407	1.00	45.72	D
ATOM	5476	CB	VAL	D	35	63.626	74.823	186.627	1.00	47.91	D
ATOM	5477	CG1	VAL	D	35	63.499	73.378	186.179	1.00	47.30	D
ATOM	5478	CG2	VAL	D	35	64.840	74.994	187.534	1.00	42.49	D
ATOM	5479	C	VAL	D	35	62.595	75.549	184.488	1.00	40.70	D
ATOM	5480	O	VAL	D	35	61.467	75.913	184.825	1.00	39.68	D
ATOM	5481	N	VAL	D	36	62.867	74.987	183.315	1.00	37.55	D
ATOM	5482	CA	VAL	D	36	61.801	74.711	182.363	1.00	38.43	D
ATOM	5483	CB	VAL	D	36	62.098	75.248	180.969	1.00	37.19	D
ATOM	5484	CG1	VAL	D	36	60.791	75.497	180.256	1.00	40.67	D
ATOM	5485	CG2	VAL	D	36	62.908	76.513	181.053	1.00	31.30	D
ATOM	5486	C	VAL	D	36	61.730	73.209	182.289	1.00	38.19	D
ATOM	5487	O	VAL	D	36	62.590	72.559	181.688	1.00	38.88	D
ATOM	5488	N	ASP	D	37	60.716	72.645	182.926	1.00	38.30	D
ATOM	5489	CA	ASP	D	37	60.581	71.198	182.935	1.00	41.83	D
ATOM	5490	CB	ASP	D	37	60.160	70.740	184.326	1.00	44.36	D
ATOM	5491	CG	ASP	D	37	60.215	69.249	184.478	1.00	53.50	D
ATOM	5492	OD1	ASP	D	37	61.242	68.645	184.072	1.00	56.96	D
ATOM	5493	OD2	ASP	D	37	59.230	68.685	185.006	1.00	61.91	D
ATOM	5494	C	ASP	D	37	59.583	70.721	181.891	1.00	37.58	D
ATOM	5495	O	ASP	D	37	58.375	70.871	182.063	1.00	40.31	D
ATOM	5496	N	LEU	D	38	60.087	70.135	180.816	1.00	33.17	D
ATOM	5497	CA	LEU	D	38	59.205	69.681	179.753	1.00	38.45	D
ATOM	5498	CB	LEU	D	38	59.944	69.736	178.421	1.00	34.29	D
ATOM	5499	CG	LEU	D	38	60.253	71.205	178.147	1.00	29.05	D
ATOM	5500	CD1	LEU	D	38	61.183	71.294	177.012	1.00	37.61	D
ATOM	5501	CD2	LEU	D	38	58.988	71.983	177.860	1.00	29.88	D
ATOM	5502	C	LEU	D	38	58.578	68.312	179.979	1.00	39.31	D
ATOM	5503	O	LEU	D	38	57.541	67.987	179.368	1.00	32.02	D
ATOM	5504	N	SER	D	39	59.201	67.540	180.875	1.00	39.30	D
ATOM	5505	CA	SER	D	39	58.735	66.204	181.245	1.00	38.41	D
ATOM	5506	CB	SER	D	39	59.584	65.624	182.364	1.00	44.05	D
ATOM	5507	OG	SER	D	39	59.134	66.126	183.617	1.00	44.75	D
ATOM	5508	C	SER	D	39	57.334	66.367	181.786	1.00	35.99	D
ATOM	5509	O	SER	D	39	56.616	65.403	182.018	1.00	37.62	D
ATOM	5510	N	THR	D	40	56.954	67.609	182.010	1.00	32.86	D
ATOM	5511	CA	THR	D	40	55.642	67.871	182.520	1.00	30.31	D
ATOM	5512	CB	THR	D	40	55.705	69.015	183.541	1.00	27.64	D
ATOM	5513	OG1	THR	D	40	55.288	68.509	184.808	1.00	35.55	D
ATOM	5514	CG2	THR	D	40	54.816	70.172	183.150	1.00	21.43	D
ATOM	5515	C	THR	D	40	54.725	68.222	181.377	1.00	30.56	D
ATOM	5516	O	THR	D	40	53.501	68.248	181.530	1.00	31.24	D
ATOM	5517	N	GLN	D	41	55.308	68.470	180.212	1.00	32.19	D
ATOM	5518	CA	GLN	D	41	54.488	68.872	179.079	1.00	36.72	D
ATOM	5519	CB	GLN	D	41	54.773	70.333	178.759	1.00	42.92	D



ATOM	5520	CG	GLN	D	41	54.345	71.270	179.864	1.00	46.49	D
ATOM	5521	CD	GLN	D	41	53.678	72.486	179.310	1.00	53.46	D
ATOM	5522	OE1	GLN	D	41	54.340	73.408	178.821	1.00	59.57	D
ATOM	5523	NE2	GLN	D	41	52.349	72.493	179.344	1.00	54.24	D
ATOM	5524	C	GLN	D	41	54.588	68.056	177.801	1.00	35.51	D
ATOM	5525	O	GLN	D	41	53.803	68.260	176.879	1.00	31.88	D
ATOM	5526	N	ILE	D	42	55.545	67.136	177.742	1.00	33.84	D
ATOM	5527	CA	ILE	D	42	55.724	66.327	176.547	1.00	32.88	D
ATOM	5528	CB	ILE	D	42	57.020	66.713	175.833	1.00	28.07	D
ATOM	5529	CG2	ILE	D	42	57.183	65.907	174.567	1.00	34.76	D
ATOM	5530	CG1	ILE	D	42	56.995	68.198	175.494	1.00	27.76	D
ATOM	5531	CD1	ILE	D	42	58.309	68.691	174.960	1.00	34.03	D
ATOM	5532	C	ILE	D	42	55.740	64.834	176.866	1.00	36.38	D
ATOM	5533	O	ILE	D	42	56.599	64.344	177.619	1.00	33.44	D
ATOM	5534	N	PHE	D	43	54.779	64.124	176.272	1.00	38.64	D
ATOM	5535	CA	PHE	D	43	54.617	62.685	176.462	1.00	38.64	D
ATOM	5536	CB	PHE	D	43	53.300	62.410	177.167	1.00	35.19	D
ATOM	5537	CG	PHE	D	43	53.176	63.105	178.470	1.00	36.76	D
ATOM	5538	CD1	PHE	D	43	52.732	64.421	178.528	1.00	35.03	D
ATOM	5539	CD2	PHE	D	43	53.560	62.462	179.649	1.00	41.65	D
ATOM	5540	CE1	PHE	D	43	52.669	65.095	179.744	1.00	36.26	D
ATOM	5541	CE2	PHE	D	43	53.505	63.121	180.871	1.00	40.83	D
ATOM	5542	CZ	PHE	D	43	53.057	64.444	180.923	1.00	37.78	D
ATOM	5543	C	PHE	D	43	54.665	61.850	175.196	1.00	40.30	D
ATOM	5544	O	PHE	D	43	54.162	62.243	174.153	1.00	44.47	D
ATOM	5545	N	CYS	D	44	55.266	60.678	175.299	1.00	40.91	D
ATOM	5546	CA	CYS	D	44	55.343	59.777	174.164	1.00	42.07	D
ATOM	5547	C	CYS	D	44	54.956	58.352	174.601	1.00	43.01	D
ATOM	5548	O	CYS	D	44	54.817	58.059	175.796	1.00	43.90	D
ATOM	5549	CB	CYS	D	44	56.756	59.778	173.595	1.00	44.51	D
ATOM	5550	SG	CYS	D	44	57.417	61.408	173.127	1.00	48.68	D
ATOM	5551	N	HIS	D	45	54.768	57.470	173.628	1.00	39.90	D
ATOM	5552	CA	HIS	D	45	54.404	56.100	173.926	1.00	36.67	D
ATOM	5553	CB	HIS	D	45	52.897	55.955	174.129	1.00	30.05	D
ATOM	5554	CG	HIS	D	45	52.105	56.141	172.877	1.00	38.40	D
ATOM	5555	CD2	HIS	D	45	52.045	55.404	171.741	1.00	40.05	D
ATOM	5556	ND1	HIS	D	45	51.307	57.242	172.659	1.00	41.79	D
ATOM	5557	CE1	HIS	D	45	50.796	57.180	171.442	1.00	43.93	D
ATOM	5558	NE2	HIS	D	45	51.229	56.074	170.863	1.00	41.62	D
ATOM	5559	C	HIS	D	45	54.826	55.249	172.756	1.00	37.41	D
ATOM	5560	O	HIS	D	45	55.002	55.753	171.648	1.00	38.92	D
ATOM	5561	N	ASN	D	46	54.997	53.959	173.026	1.00	39.62	D
ATOM	5562	CA	ASN	D	46	55.375	52.959	172.037	1.00	40.59	D
ATOM	5563	CB	ASN	D	46	56.081	51.813	172.755	1.00	42.61	D
ATOM	5564	CG	ASN	D	46	56.831	50.908	171.815	1.00	40.31	D
ATOM	5565	OD1	ASN	D	46	56.327	50.533	170.759	1.00	40.56	D
ATOM	5566	ND2	ASN	D	46	58.043	50.544	172.197	1.00	35.28	D
ATOM	5567	C	ASN	D	46	54.037	52.472	171.463	1.00	42.95	D
ATOM	5568	O	ASN	D	46	53.074	52.310	172.208	1.00	42.82	D
ATOM	5569	N	ASP	D	47	53.947	52.249	170.159	1.00	44.85	D
ATOM	5570	CA	ASP	D	47	52.670	51.790	169.602	1.00	48.92	D
ATOM	5571	CB	ASP	D	47	52.437	52.399	168.205	1.00	46.60	D
ATOM	5572	CG	ASP	D	47	51.947	53.851	168.262	1.00	48.03	D
ATOM	5573	OD1	ASP	D	47	50.909	54.120	168.904	1.00	49.27	D
ATOM	5574	OD2	ASP	D	47	52.593	54.733	167.656	1.00	47.69	D
ATOM	5575	C	ASP	D	47	52.563	50.254	169.547	1.00	49.01	D
ATOM	5576	O	ASP	D	47	51.469	49.689	169.560	1.00	47.25	D
ATOM	5577	N	TYR	D	48	53.704	49.582	169.496	1.00	48.84	D



ATOM	5578	CA	TYR	D	48	53.718	48.132	169.452	1.00	48.99	D
ATOM	5579	CB	TYR	D	48	53.971	47.651	168.024	1.00	51.60	D
ATOM	5580	CG	TYR	D	48	53.001	48.240	167.015	1.00	57.36	D
ATOM	5581	CD1	TYR	D	48	53.330	49.396	166.298	1.00	60.60	D
ATOM	5582	CE1	TYR	D	48	52.435	49.968	165.396	1.00	61.32	D
ATOM	5583	CD2	TYR	D	48	51.742	47.665	166.800	1.00	57.87	D
ATOM	5584	CE2	TYR	D	48	50.833	48.233	165.899	1.00	60.38	D
ATOM	5585	CZ	TYR	D	48	51.190	49.388	165.205	1.00	61.77	D
ATOM	5586	OH	TYR	D	48	50.298	49.994	164.354	1.00	59.47	D
ATOM	5587	C	TYR	D	48	54.800	47.634	170.393	1.00	48.38	D
ATOM	5588	O	TYR	D	48	55.802	47.055	169.964	1.00	49.69	D
ATOM	5589	N	PRO	D	49	54.600	47.856	171.701	1.00	47.71	D
ATOM	5590	CD	PRO	D	49	53.397	48.476	172.283	1.00	49.30	D
ATOM	5591	CA	PRO	D	49	55.535	47.454	172.753	1.00	50.81	D
ATOM	5592	CB	PRO	D	49	54.788	47.821	174.040	1.00	49.19	D
ATOM	5593	CG	PRO	D	49	53.348	47.848	173.634	1.00	47.87	D
ATOM	5594	C	PRO	D	49	55.991	45.997	172.719	1.00	54.81	D
ATOM	5595	O	PRO	D	49	57.189	45.727	172.621	1.00	55.51	D
ATOM	5596	N	GLU	D	50	55.036	45.067	172.780	1.00	56.17	D
ATOM	5597	CA	GLU	D	50	55.318	43.623	172.777	1.00	54.59	D
ATOM	5598	CB	GLU	D	50	54.025	42.817	172.631	1.00	47.73	D
ATOM	5599	CG	GLU	D	50	52.923	43.186	173.595	1.00	55.13	D
ATOM	5600	CD	GLU	D	50	52.230	44.484	173.218	1.00	63.88	D
ATOM	5601	OE1	GLU	D	50	52.407	44.948	172.061	1.00	63.40	D
ATOM	5602	OE2	GLU	D	50	51.497	45.033	174.073	1.00	63.47	D
ATOM	5603	C	GLU	D	50	56.302	43.090	171.732	1.00	53.44	D
ATOM	5604	O	GLU	D	50	56.875	42.023	171.925	1.00	56.75	D
ATOM	5605	N	THR	D	51	56.507	43.803	170.632	1.00	48.96	D
ATOM	5606	CA	THR	D	51	57.415	43.295	169.608	1.00	52.60	D
ATOM	5607	CB	THR	D	51	56.612	42.792	168.376	1.00	53.57	D
ATOM	5608	OG1	THR	D	51	56.331	43.879	167.477	1.00	46.96	D
ATOM	5609	CG2	THR	D	51	55.290	42.219	168.840	1.00	55.69	D
ATOM	5610	C	THR	D	51	58.437	44.339	169.156	1.00	55.47	D
ATOM	5611	O	THR	D	51	59.407	44.025	168.452	1.00	55.82	D
ATOM	5612	N	ILE	D	52	58.225	45.586	169.558	1.00	51.66	D
ATOM	5613	CA	ILE	D	52	59.145	46.627	169.163	1.00	45.39	D
ATOM	5614	CB	ILE	D	52	58.512	47.541	168.116	1.00	49.25	D
ATOM	5615	CG2	ILE	D	52	59.467	48.670	167.755	1.00	46.46	D
ATOM	5616	CG1	ILE	D	52	58.150	46.717	166.875	1.00	48.34	D
ATOM	5617	CD1	ILE	D	52	57.480	47.514	165.783	1.00	50.24	D
ATOM	5618	C	ILE	D	52	59.561	47.453	170.347	1.00	44.62	D
ATOM	5619	O	ILE	D	52	58.744	47.774	171.205	1.00	42.27	D
ATOM	5620	N	THR	D	53	60.851	47.762	170.407	1.00	45.97	D
ATOM	5621	CA	THR	D	53	61.385	48.593	171.475	1.00	48.38	D
ATOM	5622	CB	THR	D	53	62.564	47.910	172.195	1.00	50.53	D
ATOM	5623	OG1	THR	D	53	62.052	46.994	173.176	1.00	48.05	D
ATOM	5624	CG2	THR	D	53	63.447	48.948	172.885	1.00	47.27	D
ATOM	5625	C	THR	D	53	61.839	49.917	170.877	1.00	48.03	D
ATOM	5626	O	THR	D	53	62.657	49.942	169.947	1.00	44.73	D
ATOM	5627	N	ASP	D	54	61.293	51.011	171.413	1.00	50.05	D
ATOM	5628	CA	ASP	D	54	61.616	52.354	170.931	1.00	49.86	D
ATOM	5629	CB	ASP	D	54	60.355	53.232	170.937	1.00	48.25	D
ATOM	5630	CG	ASP	D	54	59.374	52.870	169.821	1.00	46.20	D
ATOM	5631	OD1	ASP	D	54	59.837	52.582	168.698	1.00	48.29	D
ATOM	5632	OD2	ASP	D	54	58.145	52.890	170.057	1.00	42.24	D
ATOM	5633	C	ASP	D	54	62.733	53.047	171.721	1.00	47.79	D
ATOM	5634	O	ASP	D	54	62.809	52.936	172.946	1.00	43.23	D
ATOM	5635	N	TYR	D	55	63.595	53.756	170.990	1.00	50.75	D



ATOM	5636	CA	TYR	D	55	64.730	54.502	171.554	1.00	51.63	D
ATOM	5637	CB	TYR	D	55	66.036	54.057	170.899	1.00	52.94	D
ATOM	5638	CG	TYR	D	55	66.308	52.580	170.991	1.00	53.68	D
ATOM	5639	CD1	TYR	D	55	66.715	51.869	169.858	1.00	51.76	D
ATOM	5640	CE1	TYR	D	55	66.948	50.507	169.908	1.00	51.50	D
ATOM	5641	CD2	TYR	D	55	66.146	51.887	172.197	1.00	50.68	D
ATOM	5642	CE2	TYR	D	55	66.380	50.514	172.265	1.00	55.22	D
ATOM	5643	CZ	TYR	D	55	66.779	49.829	171.107	1.00	54.89	D
ATOM	5644	OH	TYR	D	55	66.986	48.469	171.129	1.00	49.34	D
ATOM	5645	C	TYR	D	55	64.581	56.009	171.325	1.00	48.85	D
ATOM	5646	O	TYR	D	55	64.646	56.483	170.190	1.00	48.91	D
ATOM	5647	N	VAL	D	56	64.396	56.752	172.409	1.00	47.81	D
ATOM	5648	CA	VAL	D	56	64.241	58.198	172.338	1.00	45.40	D
ATOM	5649	CB	VAL	D	56	63.075	58.650	173.192	1.00	43.96	D
ATOM	5650	CG1	VAL	D	56	62.973	60.164	173.169	1.00	48.40	D
ATOM	5651	CG2	VAL	D	56	61.811	58.021	172.664	1.00	45.38	D
ATOM	5652	C	VAL	D	56	65.506	58.908	172.790	1.00	44.94	D
ATOM	5653	O	VAL	D	56	66.077	58.607	173.823	1.00	47.71	D
ATOM	5654	N	THR	D	57	65.915	59.897	172.021	1.00	46.85	D
ATOM	5655	CA	THR	D	57	67.150	60.612	172.292	1.00	41.59	D
ATOM	5656	CB	THR	D	57	68.178	60.122	171.271	1.00	33.45	D
ATOM	5657	OG1	THR	D	57	69.478	60.114	171.836	1.00	37.75	D
ATOM	5658	CG2	THR	D	57	68.159	61.001	170.067	1.00	24.52	D
ATOM	5659	C	THR	D	57	66.968	62.135	172.139	1.00	41.37	D
ATOM	5660	O	THR	D	57	66.090	62.570	171.394	1.00	43.18	D
ATOM	5661	N	LEU	D	58	67.773	62.938	172.841	1.00	38.63	D
ATOM	5662	CA	LEU	D	58	67.698	64.393	172.680	1.00	38.82	D
ATOM	5663	CB	LEU	D	58	68.012	65.135	173.981	1.00	38.58	D
ATOM	5664	CG	LEU	D	58	68.130	66.662	173.793	1.00	40.37	D
ATOM	5665	CD1	LEU	D	58	66.765	67.237	173.408	1.00	37.66	D
ATOM	5666	CD2	LEU	D	58	68.643	67.332	175.053	1.00	33.86	D
ATOM	5667	C	LEU	D	58	68.735	64.785	171.619	1.00	41.06	D
ATOM	5668	O	LEU	D	58	69.847	65.228	171.945	1.00	43.92	D
ATOM	5669	N	GLN	D	59	68.350	64.610	170.356	1.00	40.77	D
ATOM	5670	CA	GLN	D	59	69.179	64.900	169.181	1.00	40.87	D
ATOM	5671	CB	GLN	D	59	68.291	64.870	167.933	1.00	46.84	D
ATOM	5672	CG	GLN	D	59	68.800	64.053	166.754	1.00	58.79	D
ATOM	5673	CD	GLN	D	59	70.198	64.427	166.328	1.00	68.42	D
ATOM	5674	OE1	GLN	D	59	71.183	63.989	166.927	1.00	77.06	D
ATOM	5675	NE2	GLN	D	59	70.299	65.250	165.290	1.00	74.25	D
ATOM	5676	C	GLN	D	59	69.918	66.247	169.226	1.00	38.61	D
ATOM	5677	O	GLN	D	59	71.114	66.317	168.953	1.00	35.55	D
ATOM	5678	N	ARG	D	60	69.187	67.308	169.559	1.00	36.04	D
ATOM	5679	CA	ARG	D	60	69.741	68.651	169.618	1.00	36.19	D
ATOM	5680	CB	ARG	D	60	69.805	69.229	168.199	1.00	37.08	D
ATOM	5681	CG	ARG	D	60	70.596	70.520	168.047	1.00	47.03	D
ATOM	5682	CD	ARG	D	60	70.500	71.078	166.621	1.00	56.12	D
ATOM	5683	NE	ARG	D	60	70.137	70.049	165.637	1.00	72.98	D
ATOM	5684	CZ	ARG	D	60	70.899	69.003	165.292	1.00	77.04	D
ATOM	5685	NH1	ARG	D	60	72.098	68.821	165.843	1.00	76.99	D
ATOM	5686	NH2	ARG	D	60	70.453	68.121	164.399	1.00	73.66	D
ATOM	5687	C	ARG	D	60	68.887	69.552	170.519	1.00	36.39	D
ATOM	5688	O	ARG	D	60	67.696	69.320	170.698	1.00	43.92	D
ATOM	5689	N	GLY	D	61	69.506	70.573	171.092	1.00	33.53	D
ATOM	5690	CA	GLY	D	61	68.804	71.503	171.954	1.00	31.15	D
ATOM	5691	C	GLY	D	61	69.350	72.865	171.592	1.00	33.73	D
ATOM	5692	O	GLY	D	61	70.561	73.062	171.608	1.00	34.33	D
ATOM	5693	N	SER	D	62	68.471	73.805	171.260	1.00	34.12	D



ATOM	5694	CA	SER	D	62	68.920	75.122	170.852	1.00	33.13	D
ATOM	5695	CB	SER	D	62	68.759	75.270	169.341	1.00	34.81	D
ATOM	5696	OG	SER	D	62	69.546	74.312	168.661	1.00	33.21	D
ATOM	5697	C	SER	D	62	68.189	76.239	171.542	1.00	35.12	D
ATOM	5698	O	SER	D	62	66.986	76.143	171.778	1.00	40.21	D
ATOM	5699	N	ALA	D	63	68.924	77.315	171.825	1.00	34.52	D
ATOM	5700	CA	ALA	D	63	68.384	78.487	172.514	1.00	29.48	D
ATOM	5701	CB	ALA	D	63	69.369	78.960	173.563	1.00	29.03	D
ATOM	5702	C	ALA	D	63	68.058	79.627	171.564	1.00	26.39	D
ATOM	5703	O	ALA	D	63	68.665	79.757	170.520	1.00	29.01	D
ATOM	5704	N	TYR	D	64	67.098	80.456	171.948	1.00	25.45	D
ATOM	5705	CA	TYR	D	64	66.668	81.586	171.141	1.00	25.29	D
ATOM	5706	CB	TYR	D	64	65.439	81.213	170.296	1.00	29.09	D
ATOM	5707	CG	TYR	D	64	65.740	80.177	169.244	1.00	34.22	D
ATOM	5708	CD1	TYR	D	64	65.695	78.812	169.540	1.00	37.16	D
ATOM	5709	CE1	TYR	D	64	66.087	77.861	168.599	1.00	40.42	D
ATOM	5710	CD2	TYR	D	64	66.171	80.559	167.984	1.00	34.69	D
ATOM	5711	CE2	TYR	D	64	66.562	79.625	167.045	1.00	35.37	D
ATOM	5712	CZ	TYR	D	64	66.523	78.286	167.352	1.00	42.68	D
ATOM	5713	OH	TYR	D	64	66.941	77.379	166.413	1.00	52.45	D
ATOM	5714	C	TYR	D	64	66.336	82.792	171.997	1.00	26.55	D
ATOM	5715	O	TYR	D	64	66.082	82.662	173.199	1.00	30.08	D
ATOM	5716	N	GLY	D	65	66.339	83.963	171.365	1.00	24.96	D
ATOM	5717	CA	GLY	D	65	66.036	85.197	172.060	1.00	24.91	D
ATOM	5718	C	GLY	D	65	66.800	85.352	173.358	1.00	28.86	D
ATOM	5719	O	GLY	D	65	68.014	85.060	173.445	1.00	28.91	D
ATOM	5720	N	GLY	D	66	66.075	85.792	174.381	1.00	25.34	D
ATOM	5721	CA	GLY	D	66	66.683	86.018	175.674	1.00	27.04	D
ATOM	5722	C	GLY	D	66	67.464	84.840	176.183	1.00	26.29	D
ATOM	5723	O	GLY	D	66	68.574	84.998	176.636	1.00	32.30	D
ATOM	5724	N	VAL	D	67	66.889	83.653	176.112	1.00	27.48	D
ATOM	5725	CA	VAL	D	67	67.585	82.481	176.599	1.00	30.59	D
ATOM	5726	CB	VAL	D	67	66.864	81.199	176.189	1.00	28.05	D
ATOM	5727	CG1	VAL	D	67	67.796	80.003	176.374	1.00	23.61	D
ATOM	5728	CG2	VAL	D	67	65.605	81.023	177.034	1.00	18.84	D
ATOM	5729	C	VAL	D	67	69.009	82.411	176.083	1.00	34.05	D
ATOM	5730	O	VAL	D	67	69.932	82.030	176.803	1.00	36.67	D
ATOM	5731	N	LEU	D	68	69.169	82.796	174.831	1.00	36.19	D
ATOM	5732	CA	LEU	D	68	70.454	82.764	174.155	1.00	38.03	D
ATOM	5733	CB	LEU	D	68	70.189	82.881	172.663	1.00	38.26	D
ATOM	5734	CG	LEU	D	68	71.270	82.612	171.633	1.00	32.92	D
ATOM	5735	CD1	LEU	D	68	71.832	81.215	171.803	1.00	26.29	D
ATOM	5736	CD2	LEU	D	68	70.642	82.780	170.256	1.00	29.24	D
ATOM	5737	C	LEU	D	68	71.432	83.856	174.584	1.00	40.10	D
ATOM	5738	O	LEU	D	68	72.642	83.638	174.660	1.00	41.49	D
ATOM	5739	N	SER	D	69	70.911	85.033	174.877	1.00	38.23	D
ATOM	5740	CA	SER	D	69	71.784	86.133	175.237	1.00	38.34	D
ATOM	5741	CB	SER	D	69	71.292	87.411	174.560	1.00	37.73	D
ATOM	5742	OG	SER	D	69	69.954	87.698	174.938	1.00	34.57	D
ATOM	5743	C	SER	D	69	71.955	86.406	176.716	1.00	37.45	D
ATOM	5744	O	SER	D	69	72.970	86.968	177.113	1.00	36.78	D
ATOM	5745	N	ASN	D	70	70.977	86.003	177.526	1.00	35.91	D
ATOM	5746	CA	ASN	D	70	71.008	86.259	178.962	1.00	35.34	D
ATOM	5747	CB	ASN	D	70	69.714	86.954	179.377	1.00	34.25	D
ATOM	5748	CG	ASN	D	70	69.423	88.164	178.525	1.00	38.04	D
ATOM	5749	OD1	ASN	D	70	70.343	88.830	178.063	1.00	46.18	D
ATOM	5750	ND2	ASN	D	70	68.147	88.465	178.318	1.00	44.74	D
ATOM	5751	C	ASN	D	70	71.237	85.085	179.897	1.00	38.20	D



ATOM	5752	O	ASN	D	70	71.270	85.265	181.118	1.00	42.79	D
ATOM	5753	N	PHE	D	71	71.407	83.889	179.360	1.00	36.65	D
ATOM	5754	CA	PHE	D	71	71.577	82.755	180.245	1.00	33.92	D
ATOM	5755	CB	PHE	D	71	70.283	81.941	180.307	1.00	28.49	D
ATOM	5756	CG	PHE	D	71	69.114	82.681	180.876	1.00	25.93	D
ATOM	5757	CD1	PHE	D	71	68.430	83.626	180.121	1.00	30.86	D
ATOM	5758	CD2	PHE	D	71	68.683	82.421	182.179	1.00	20.33	D
ATOM	5759	CE1	PHE	D	71	67.310	84.311	180.675	1.00	39.06	D
ATOM	5760	CE2	PHE	D	71	67.585	83.086	182.735	1.00	22.00	D
ATOM	5761	CZ	PHE	D	71	66.893	84.032	181.988	1.00	24.40	D
ATOM	5762	C	PHE	D	71	72.701	81.820	179.857	1.00	36.97	D
ATOM	5763	O	PHE	D	71	73.218	81.851	178.731	1.00	36.04	D
ATOM	5764	N	SER	D	72	73.084	80.996	180.822	1.00	35.89	D
ATOM	5765	CA	SER	D	72	74.091	79.973	180.613	1.00	41.93	D
ATOM	5766	CB	SER	D	72	75.382	80.267	181.389	1.00	43.25	D
ATOM	5767	OG	SER	D	72	75.176	80.196	182.787	1.00	51.92	D
ATOM	5768	C	SER	D	72	73.354	78.791	181.220	1.00	42.70	D
ATOM	5769	O	SER	D	72	72.686	78.933	182.248	1.00	44.36	D
ATOM	5770	N	GLY	D	73	73.422	77.628	180.602	1.00	42.36	D
ATOM	5771	CA	GLY	D	73	72.669	76.563	181.213	1.00	43.37	D
ATOM	5772	C	GLY	D	73	72.949	75.156	180.797	1.00	41.31	D
ATOM	5773	O	GLY	D	73	73.766	74.882	179.908	1.00	37.82	D
ATOM	5774	N	THR	D	74	72.245	74.255	181.467	1.00	40.50	D
ATOM	5775	CA	THR	D	74	72.396	72.847	181.180	1.00	45.58	D
ATOM	5776	CB	THR	D	74	73.000	72.067	182.386	1.00	47.49	D
ATOM	5777	OG1	THR	D	74	72.059	72.057	183.467	1.00	51.70	D
ATOM	5778	CG2	THR	D	74	74.317	72.704	182.846	1.00	38.61	D
ATOM	5779	C	THR	D	74	71.050	72.246	180.852	1.00	42.69	D
ATOM	5780	O	THR	D	74	69.998	72.856	181.087	1.00	35.56	D
ATOM	5781	N	VAL	D	75	71.106	71.052	180.275	1.00	44.17	D
ATOM	5782	CA	VAL	D	75	69.900	70.312	179.941	1.00	44.78	D
ATOM	5783	CB	VAL	D	75	69.753	70.057	178.396	1.00	44.61	D
ATOM	5784	CG1	VAL	D	75	70.974	69.306	177.841	1.00	43.76	D
ATOM	5785	CG2	VAL	D	75	68.481	69.280	178.128	1.00	33.87	D
ATOM	5786	C	VAL	D	75	70.007	68.988	180.676	1.00	43.56	D
ATOM	5787	O	VAL	D	75	71.003	68.266	180.539	1.00	37.52	D
ATOM	5788	N	LYS	D	76	69.002	68.697	181.491	1.00	43.49	D
ATOM	5789	CA	LYS	D	76	68.990	67.445	182.220	1.00	48.22	D
ATOM	5790	CB	LYS	D	76	68.468	67.648	183.645	1.00	52.15	D
ATOM	5791	CG	LYS	D	76	68.795	66.480	184.569	1.00	59.05	D
ATOM	5792	CD	LYS	D	76	68.332	66.715	186.003	1.00	65.92	D
ATOM	5793	CE	LYS	D	76	68.776	65.564	186.913	1.00	68.75	D
ATOM	5794	NZ	LYS	D	76	68.367	65.769	188.337	1.00	72.96	D
ATOM	5795	C	LYS	D	76	68.098	66.447	181.480	1.00	50.18	D
ATOM	5796	O	LYS	D	76	66.868	66.562	181.500	1.00	50.92	D
ATOM	5797	N	TYR	D	77	68.724	65.473	180.823	1.00	47.77	D
ATOM	5798	CA	TYR	D	77	67.984	64.461	180.093	1.00	46.46	D
ATOM	5799	CB	TYR	D	77	68.514	64.302	178.676	1.00	38.80	D
ATOM	5800	CG	TYR	D	77	67.678	63.337	177.868	1.00	42.71	D
ATOM	5801	CD1	TYR	D	77	66.305	63.528	177.735	1.00	40.46	D
ATOM	5802	CE1	TYR	D	77	65.536	62.681	176.949	1.00	43.60	D
ATOM	5803	CD2	TYR	D	77	68.260	62.258	177.198	1.00	42.40	D
ATOM	5804	CE2	TYR	D	77	67.500	61.398	176.403	1.00	34.47	D
ATOM	5805	CZ	TYR	D	77	66.135	61.620	176.277	1.00	44.63	D
ATOM	5806	OH	TYR	D	77	65.363	60.837	175.431	1.00	45.13	D
ATOM	5807	C	TYR	D	77	68.036	63.095	180.733	1.00	50.05	D
ATOM	5808	O	TYR	D	77	69.043	62.401	180.608	1.00	51.74	D
ATOM	5809	N	SER	D	78	66.956	62.695	181.396	1.00	52.61	D



ATOM	5810	CA	SER	D	78	66.904	61.368	181.996	1.00	55.05	D
ATOM	5811	CB	SER	D	78	67.067	60.303	180.889	1.00	54.80	D
ATOM	5812	OG	SER	D	78	66.889	58.971	181.359	1.00	52.93	D
ATOM	5813	C	SER	D	78	67.972	61.172	183.063	1.00	58.11	D
ATOM	5814	O	SER	D	78	68.764	60.236	182.990	1.00	62.64	D
ATOM	5815	N	GLY	D	79	68.013	62.059	184.047	1.00	59.15	D
ATOM	5816	CA	GLY	D	79	69.001	61.898	185.100	1.00	61.56	D
ATOM	5817	C	GLY	D	79	70.366	62.536	184.901	1.00	62.86	D
ATOM	5818	O	GLY	D	79	71.004	62.903	185.886	1.00	65.64	D
ATOM	5819	N	SER	D	80	70.825	62.665	183.656	1.00	61.18	D
ATOM	5820	CA	SER	D	80	72.128	63.281	183.378	1.00	60.35	D
ATOM	5821	CB	SER	D	80	72.915	62.431	182.389	1.00	57.76	D
ATOM	5822	OG	SER	D	80	73.236	61.193	182.977	1.00	66.01	D
ATOM	5823	C	SER	D	80	72.022	64.708	182.834	1.00	59.17	D
ATOM	5824	O	SER	D	80	70.971	65.112	182.335	1.00	58.18	D
ATOM	5825	N	SER	D	81	73.115	65.467	182.929	1.00	56.61	D
ATOM	5826	CA	SER	D	81	73.119	66.848	182.450	1.00	50.07	D
ATOM	5827	CB	SER	D	81	73.371	67.836	183.598	1.00	51.95	D
ATOM	5828	OG	SER	D	81	72.155	68.372	184.107	1.00	47.34	D
ATOM	5829	C	SER	D	81	74.120	67.088	181.344	1.00	46.16	D
ATOM	5830	O	SER	D	81	75.148	66.432	181.247	1.00	41.56	D
ATOM	5831	N	TYR	D	82	73.793	68.036	180.485	1.00	48.76	D
ATOM	5832	CA	TYR	D	82	74.655	68.351	179.363	1.00	49.74	D
ATOM	5833	CB	TYR	D	82	74.222	67.575	178.099	1.00	50.52	D
ATOM	5834	CG	TYR	D	82	73.962	66.098	178.315	1.00	51.28	D
ATOM	5835	CD1	TYR	D	82	72.837	65.661	179.022	1.00	49.16	D
ATOM	5836	CE1	TYR	D	82	72.626	64.310	179.286	1.00	53.58	D
ATOM	5837	CD2	TYR	D	82	74.867	65.137	177.864	1.00	55.30	D
ATOM	5838	CE2	TYR	D	82	74.664	63.767	178.117	1.00	52.76	D
ATOM	5839	CZ	TYR	D	82	73.544	63.362	178.831	1.00	57.08	D
ATOM	5840	OH	TYR	D	82	73.340	62.017	179.096	1.00	59.70	D
ATOM	5841	C	TYR	D	82	74.565	69.846	179.101	1.00	47.56	D
ATOM	5842	O	TYR	D	82	73.615	70.528	179.525	1.00	47.60	D
ATOM	5843	N	PRO	D	83	75.558	70.376	178.395	1.00	42.33	D
ATOM	5844	CD	PRO	D	83	76.766	69.660	177.968	1.00	37.77	D
ATOM	5845	CA	PRO	D	83	75.634	71.793	178.049	1.00	42.94	D
ATOM	5846	CB	PRO	D	83	76.981	71.898	177.347	1.00	39.08	D
ATOM	5847	CG	PRO	D	83	77.759	70.761	177.929	1.00	43.25	D
ATOM	5848	C	PRO	D	83	74.489	72.203	177.132	1.00	44.94	D
ATOM	5849	O	PRO	D	83	74.215	71.528	176.141	1.00	48.59	D
ATOM	5850	N	PHE	D	84	73.819	73.298	177.466	1.00	44.30	D
ATOM	5851	CA	PHE	D	84	72.733	73.804	176.630	1.00	44.32	D
ATOM	5852	CB	PHE	D	84	71.386	73.671	177.342	1.00	42.78	D
ATOM	5853	CG	PHE	D	84	70.231	74.240	176.562	1.00	39.68	D
ATOM	5854	CD1	PHE	D	84	69.666	73.528	175.515	1.00	38.18	D
ATOM	5855	CD2	PHE	D	84	69.714	75.497	176.872	1.00	38.62	D
ATOM	5856	CE1	PHE	D	84	68.605	74.062	174.793	1.00	42.76	D
ATOM	5857	CE2	PHE	D	84	68.652	76.036	176.152	1.00	37.07	D
ATOM	5858	CZ	PHE	D	84	68.096	75.319	175.115	1.00	35.45	D
ATOM	5859	C	PHE	D	84	72.992	75.280	176.306	1.00	46.00	D
ATOM	5860	O	PHE	D	84	73.184	76.104	177.213	1.00	48.06	D
ATOM	5861	N	PRO	D	85	72.967	75.649	175.011	1.00	45.37	D
ATOM	5862	CD	PRO	D	85	73.201	77.059	174.655	1.00	43.57	D
ATOM	5863	CA	PRO	D	85	72.737	74.855	173.800	1.00	43.76	D
ATOM	5864	CB	PRO	D	85	73.202	75.794	172.699	1.00	39.35	D
ATOM	5865	CG	PRO	D	85	72.733	77.111	173.210	1.00	42.33	D
ATOM	5866	C	PRO	D	85	73.502	73.550	173.819	1.00	43.70	D
ATOM	5867	O	PRO	D	85	74.603	73.494	174.350	1.00	48.50	D



ATOM	5868	N	THR	D	86	72.924	72.502	173.247	1.00	40.19	D
ATOM	5869	CA	THR	D	86	73.575	71.202	173.247	1.00	40.13	D
ATOM	5870	CB	THR	D	86	72.585	70.096	172.924	1.00	36.77	D
ATOM	5871	OG1	THR	D	86	72.165	70.212	171.560	1.00	38.01	D
ATOM	5872	CG2	THR	D	86	71.389	70.193	173.832	1.00	36.13	D
ATOM	5873	C	THR	D	86	74.706	71.147	172.241	1.00	44.65	D
ATOM	5874	O	THR	D	86	74.745	71.933	171.299	1.00	45.24	D
ATOM	5875	N	THR	D	87	75.619	70.201	172.440	1.00	50.30	D
ATOM	5876	CA	THR	D	87	76.779	70.044	171.553	1.00	53.99	D
ATOM	5877	CB	THR	D	87	78.075	70.379	172.296	1.00	53.50	D
ATOM	5878	OG1	THR	D	87	78.015	69.825	173.619	1.00	60.15	D
ATOM	5879	CG2	THR	D	87	78.265	71.872	172.377	1.00	54.91	D
ATOM	5880	C	THR	D	87	76.938	68.641	170.967	1.00	55.08	D
ATOM	5881	O	THR	D	87	77.770	68.430	170.091	1.00	52.17	D
ATOM	5882	N	SER	D	88	76.141	67.692	171.457	1.00	57.20	D
ATOM	5883	CA	SER	D	88	76.193	66.312	170.988	1.00	55.61	D
ATOM	5884	CB	SER	D	88	77.238	65.528	171.787	1.00	57.14	D
ATOM	5885	OG	SER	D	88	76.783	65.270	173.108	1.00	56.47	D
ATOM	5886	C	SER	D	88	74.839	65.634	171.166	1.00	54.36	D
ATOM	5887	O	SER	D	88	74.034	66.053	171.996	1.00	50.10	D
ATOM	5888	N	GLU	D	89	74.587	64.588	170.382	1.00	55.43	D
ATOM	5889	CA	GLU	D	89	73.340	63.856	170.523	1.00	52.86	D
ATOM	5890	CB	GLU	D	89	73.093	62.907	169.348	1.00	53.88	D
ATOM	5891	CG	GLU	D	89	72.063	61.822	169.666	1.00	51.32	D
ATOM	5892	CD	GLU	D	89	71.461	61.186	168.432	1.00	53.86	D
ATOM	5893	OE1	GLU	D	89	72.194	60.925	167.457	1.00	56.99	D
ATOM	5894	OE2	GLU	D	89	70.246	60.932	168.444	1.00	53.32	D
ATOM	5895	C	GLU	D	89	73.471	63.063	171.810	1.00	50.22	D
ATOM	5896	O	GLU	D	89	74.441	62.346	172.027	1.00	51.19	D
ATOM	5897	N	THR	D	90	72.472	63.214	172.656	1.00	48.83	D
ATOM	5898	CA	THR	D	90	72.413	62.578	173.952	1.00	46.67	D
ATOM	5899	CB	THR	D	90	71.230	63.159	174.715	1.00	46.49	D
ATOM	5900	OG1	THR	D	90	71.625	63.440	176.056	1.00	52.22	D
ATOM	5901	CG2	THR	D	90	70.055	62.201	174.694	1.00	36.21	D
ATOM	5902	C	THR	D	90	72.278	61.061	173.895	1.00	46.92	D
ATOM	5903	O	THR	D	90	72.067	60.494	172.836	1.00	46.69	D
ATOM	5904	N	PRO	D	91	72.439	60.382	175.044	1.00	51.57	D
ATOM	5905	CD	PRO	D	91	73.078	60.888	176.273	1.00	53.12	D
ATOM	5906	CA	PRO	D	91	72.315	58.919	175.099	1.00	52.16	D
ATOM	5907	CB	PRO	D	91	72.819	58.587	176.505	1.00	52.22	D
ATOM	5908	CG	PRO	D	91	73.813	59.670	176.774	1.00	50.27	D
ATOM	5909	C	PRO	D	91	70.838	58.567	174.907	1.00	49.74	D
ATOM	5910	O	PRO	D	91	69.976	59.420	175.104	1.00	50.75	D
ATOM	5911	N	ARG	D	92	70.542	57.319	174.553	1.00	50.26	D
ATOM	5912	CA	ARG	D	92	69.154	56.914	174.308	1.00	52.79	D
ATOM	5913	CB	ARG	D	92	69.088	55.979	173.087	1.00	55.32	D
ATOM	5914	CG	ARG	D	92	69.893	54.691	173.189	1.00	62.97	D
ATOM	5915	CD	ARG	D	92	69.619	53.766	171.989	1.00	64.34	D
ATOM	5916	NE	ARG	D	92	70.121	52.393	172.157	1.00	69.97	D
ATOM	5917	CZ	ARG	D	92	70.018	51.666	173.275	1.00	70.74	D
ATOM	5918	NH1	ARG	D	92	69.440	52.168	174.363	1.00	71.05	D
ATOM	5919	NH2	ARG	D	92	70.468	50.417	173.299	1.00	67.54	D
ATOM	5920	C	ARG	D	92	68.357	56.289	175.454	1.00	50.32	D
ATOM	5921	O	ARG	D	92	68.839	55.396	176.137	1.00	57.68	D
ATOM	5922	N	VAL	D	93	67.134	56.786	175.651	1.00	43.49	D
ATOM	5923	CA	VAL	D	93	66.205	56.291	176.666	1.00	39.02	D
ATOM	5924	CB	VAL	D	93	65.383	57.419	177.288	1.00	36.13	D
ATOM	5925	CG1	VAL	D	93	64.375	56.853	178.259	1.00	34.17	D



ATOM	5926	CG2	VAL	D	93	66.280	58.383	177.989	1.00	46.18	D
ATOM	5927	C	VAL	D	93	65.226	55.376	175.937	1.00	41.91	D
ATOM	5928	O	VAL	D	93	64.966	55.582	174.747	1.00	44.04	D
ATOM	5929	N	VAL	D	94	64.672	54.375	176.622	1.00	41.51	D
ATOM	5930	CA	VAL	D	94	63.740	53.487	175.932	1.00	40.64	D
ATOM	5931	CB	VAL	D	94	64.118	51.970	176.038	1.00	37.90	D
ATOM	5932	CG1	VAL	D	94	65.632	51.777	175.893	1.00	35.27	D
ATOM	5933	CG2	VAL	D	94	63.571	51.379	177.314	1.00	28.24	D
ATOM	5934	C	VAL	D	94	62.299	53.624	176.376	1.00	41.96	D
ATOM	5935	O	VAL	D	94	61.998	53.838	177.551	1.00	37.16	D
ATOM	5936	N	TYR	D	95	61.421	53.508	175.386	1.00	45.24	D
ATOM	5937	CA	TYR	D	95	59.986	53.571	175.571	1.00	44.43	D
ATOM	5938	CB	TYR	D	95	59.386	54.685	174.704	1.00	41.75	D
ATOM	5939	CG	TYR	D	95	59.600	56.053	175.290	1.00	38.12	D
ATOM	5940	CD1	TYR	D	95	60.864	56.619	175.324	1.00	32.37	D
ATOM	5941	CE1	TYR	D	95	61.088	57.818	175.956	1.00	27.99	D
ATOM	5942	CD2	TYR	D	95	58.550	56.738	175.903	1.00	40.50	D
ATOM	5943	CE2	TYR	D	95	58.764	57.944	176.544	1.00	37.43	D
ATOM	5944	CZ	TYR	D	95	60.040	58.474	176.568	1.00	39.02	D
ATOM	5945	OH	TYR	D	95	60.286	59.657	177.231	1.00	49.00	D
ATOM	5946	C	TYR	D	95	59.426	52.213	175.159	1.00	45.02	D
ATOM	5947	O	TYR	D	95	59.642	51.752	174.022	1.00	45.31	D
ATOM	5948	N	ASN	D	96	58.723	51.583	176.097	1.00	39.92	D
ATOM	5949	CA	ASN	D	96	58.121	50.280	175.877	1.00	34.46	D
ATOM	5950	CB	ASN	D	96	59.000	49.200	176.455	1.00	34.45	D
ATOM	5951	CG	ASN	D	96	59.684	49.646	177.705	1.00	41.54	D
ATOM	5952	OD1	ASN	D	96	60.871	49.969	177.679	1.00	53.18	D
ATOM	5953	ND2	ASN	D	96	58.945	49.695	178.815	1.00	41.57	D
ATOM	5954	C	ASN	D	96	56.762	50.165	176.515	1.00	35.83	D
ATOM	5955	O	ASN	D	96	56.546	49.345	177.393	1.00	38.84	D
ATOM	5956	N	SER	D	97	55.830	50.986	176.077	1.00	34.76	D
ATOM	5957	CA	SER	D	97	54.501	50.912	176.626	1.00	33.17	D
ATOM	5958	CB	SER	D	97	54.511	51.299	178.105	1.00	20.43	D
ATOM	5959	OG	SER	D	97	53.213	51.720	178.513	1.00	24.85	D
ATOM	5960	C	SER	D	97	53.593	51.828	175.835	1.00	35.40	D
ATOM	5961	O	SER	D	97	54.011	52.890	175.386	1.00	35.61	D
ATOM	5962	N	ARG	D	98	52.355	51.394	175.638	1.00	39.41	D
ATOM	5963	CA	ARG	D	98	51.395	52.195	174.907	1.00	39.57	D
ATOM	5964	CB	ARG	D	98	50.166	51.364	174.517	1.00	43.38	D
ATOM	5965	CG	ARG	D	98	50.431	50.285	173.475	1.00	51.67	D
ATOM	5966	CD	ARG	D	98	49.122	49.691	172.928	1.00	58.46	D
ATOM	5967	NE	ARG	D	98	49.356	48.745	171.834	1.00	64.42	D
ATOM	5968	CZ	ARG	D	98	49.885	47.532	171.984	1.00	69.22	D
ATOM	5969	NH1	ARG	D	98	50.238	47.095	173.190	1.00	68.11	D
ATOM	5970	NH2	ARG	D	98	50.072	46.754	170.925	1.00	72.50	D
ATOM	5971	C	ARG	D	98	50.993	53.317	175.833	1.00	40.32	D
ATOM	5972	O	ARG	D	98	50.352	54.274	175.421	1.00	44.21	D
ATOM	5973	N	THR	D	99	51.381	53.201	177.096	1.00	43.11	D
ATOM	5974	CA	THR	D	99	51.057	54.234	178.069	1.00	48.49	D
ATOM	5975	CB	THR	D	99	51.195	53.716	179.491	1.00	47.77	D
ATOM	5976	OG1	THR	D	99	50.508	52.467	179.609	1.00	49.42	D
ATOM	5977	CG2	THR	D	99	50.590	54.711	180.461	1.00	46.69	D
ATOM	5978	C	THR	D	99	51.974	55.450	177.920	1.00	50.98	D
ATOM	5979	O	THR	D	99	53.208	55.310	177.861	1.00	50.05	D
ATOM	5980	N	ASP	D	100	51.371	56.638	177.864	1.00	50.38	D
ATOM	5981	CA	ASP	D	100	52.141	57.867	177.725	1.00	51.36	D
ATOM	5982	CB	ASP	D	100	51.230	59.091	177.631	1.00	54.66	D
ATOM	5983	CG	ASP	D	100	50.650	59.289	176.248	1.00	59.85	D



ATOM	5984	OD1	ASP	D	100	51.330	58.949	175.249	1.00	59.61	D
ATOM	5985	OD2	ASP	D	100	49.518	59.810	176.165	1.00	57.94	D
ATOM	5986	C	ASP	D	100	53.099	58.088	178.879	1.00	50.93	D
ATOM	5987	O	ASP	D	100	52.684	58.337	180.000	1.00	49.74	D
ATOM	5988	N	LYS	D	101	54.386	58.002	178.578	1.00	53.17	D
ATOM	5989	CA	LYS	D	101	55.447	58.221	179.545	1.00	51.84	D
ATOM	5990	CB	LYS	D	101	56.544	57.170	179.363	1.00	54.60	D
ATOM	5991	CG	LYS	D	101	57.883	57.517	180.006	1.00	60.79	D
ATOM	5992	CD	LYS	D	101	58.895	56.406	179.789	1.00	60.46	D
ATOM	5993	CE	LYS	D	101	60.217	56.724	180.447	1.00	60.70	D
ATOM	5994	NZ	LYS	D	101	61.105	55.546	180.307	1.00	60.74	D
ATOM	5995	C	LYS	D	101	55.990	59.615	179.226	1.00	49.53	D
ATOM	5996	O	LYS	D	101	55.843	60.093	178.103	1.00	43.87	D
ATOM	5997	N	PRO	D	102	56.603	60.293	180.215	1.00	50.95	D
ATOM	5998	CD	PRO	D	102	56.554	60.055	181.666	1.00	51.41	D
ATOM	5999	CA	PRO	D	102	57.138	61.633	179.952	1.00	48.65	D
ATOM	6000	CB	PRO	D	102	57.318	62.223	181.358	1.00	48.03	D
ATOM	6001	CG	PRO	D	102	56.336	61.456	182.187	1.00	52.32	D
ATOM	6002	C	PRO	D	102	58.456	61.574	179.202	1.00	42.44	D
ATOM	6003	O	PRO	D	102	59.088	60.528	179.111	1.00	42.74	D
ATOM	6004	N	TRP	D	103	58.842	62.700	178.631	1.00	37.59	D
ATOM	6005	CA	TRP	D	103	60.113	62.806	177.935	1.00	37.08	D
ATOM	6006	CB	TRP	D	103	59.891	63.519	176.604	1.00	30.32	D
ATOM	6007	CG	TRP	D	103	61.104	63.612	175.767	1.00	30.53	D
ATOM	6008	CD2	TRP	D	103	61.554	64.766	175.056	1.00	26.12	D
ATOM	6009	CE2	TRP	D	103	62.738	64.405	174.378	1.00	19.41	D
ATOM	6010	CE3	TRP	D	103	61.070	66.075	174.925	1.00	26.01	D
ATOM	6011	CD1	TRP	D	103	62.007	62.619	175.503	1.00	27.90	D
ATOM	6012	NE1	TRP	D	103	62.992	63.088	174.668	1.00	22.50	D
ATOM	6013	CZ2	TRP	D	103	63.450	65.307	173.581	1.00	17.75	D
ATOM	6014	CZ3	TRP	D	103	61.785	66.971	174.129	1.00	24.48	D
ATOM	6015	CH2	TRP	D	103	62.959	66.578	173.470	1.00	16.99	D
ATOM	6016	C	TRP	D	103	60.889	63.666	178.961	1.00	37.08	D
ATOM	6017	O	TRP	D	103	60.713	64.893	179.043	1.00	35.25	D
ATOM	6018	N	PRO	D	104	61.725	63.009	179.784	1.00	35.50	D
ATOM	6019	CD	PRO	D	104	62.203	61.650	179.464	1.00	35.72	D
ATOM	6020	CA	PRO	D	104	62.546	63.587	180.848	1.00	31.52	D
ATOM	6021	CB	PRO	D	104	63.165	62.360	181.483	1.00	25.01	D
ATOM	6022	CG	PRO	D	104	63.458	61.520	180.310	1.00	27.01	D
ATOM	6023	C	PRO	D	104	63.585	64.588	180.369	1.00	30.56	D
ATOM	6024	O	PRO	D	104	64.766	64.267	180.236	1.00	32.35	D
ATOM	6025	N	VAL	D	105	63.124	65.803	180.111	1.00	27.61	D
ATOM	6026	CA	VAL	D	105	63.981	66.870	179.653	1.00	26.71	D
ATOM	6027	CB	VAL	D	105	63.753	67.211	178.164	1.00	26.67	D
ATOM	6028	CG1	VAL	D	105	64.776	68.243	177.714	1.00	23.05	D
ATOM	6029	CG2	VAL	D	105	63.866	65.984	177.324	1.00	27.52	D
ATOM	6030	C	VAL	D	105	63.630	68.097	180.457	1.00	29.50	D
ATOM	6031	O	VAL	D	105	62.447	68.417	180.635	1.00	25.92	D
ATOM	6032	N	ALA	D	106	64.662	68.770	180.958	1.00	33.08	D
ATOM	6033	CA	ALA	D	106	64.467	69.995	181.718	1.00	35.06	D
ATOM	6034	CB	ALA	D	106	64.361	69.706	183.184	1.00	34.44	D
ATOM	6035	C	ALA	D	106	65.632	70.926	181.450	1.00	37.67	D
ATOM	6036	O	ALA	D	106	66.787	70.499	181.335	1.00	37.45	D
ATOM	6037	N	LEU	D	107	65.296	72.202	181.319	1.00	40.17	D
ATOM	6038	CA	LEU	D	107	66.262	73.258	181.074	1.00	41.87	D
ATOM	6039	CB	LEU	D	107	65.682	74.291	180.100	1.00	38.48	D
ATOM	6040	CG	LEU	D	107	66.105	74.215	178.627	1.00	38.10	D
ATOM	6041	CD1	LEU	D	107	66.346	72.787	178.187	1.00	31.73	D



ATOM	6042	CD2	LEU	D	107	65.047	74.879	177.781	1.00	30.60	D
ATOM	6043	C	LEU	D	107	66.551	73.929	182.397	1.00	41.81	D
ATOM	6044	O	LEU	D	107	65.630	74.287	183.131	1.00	42.43	D
ATOM	6045	N	TYR	D	108	67.832	74.056	182.716	1.00	44.52	D
ATOM	6046	CA	TYR	D	108	68.270	74.728	183.938	1.00	45.80	D
ATOM	6047	CB	TYR	D	108	69.165	73.817	184.772	1.00	44.83	D
ATOM	6048	CG	TYR	D	108	68.361	72.833	185.572	1.00	50.88	D
ATOM	6049	CD1	TYR	D	108	68.100	71.555	185.085	1.00	57.96	D
ATOM	6050	CE1	TYR	D	108	67.299	70.663	185.799	1.00	63.01	D
ATOM	6051	CD2	TYR	D	108	67.804	73.200	186.793	1.00	53.14	D
ATOM	6052	CE2	TYR	D	108	67.002	72.325	187.515	1.00	58.90	D
ATOM	6053	CZ	TYR	D	108	66.749	71.054	187.016	1.00	63.77	D
ATOM	6054	OH	TYR	D	108	65.951	70.174	187.730	1.00	65.26	D
ATOM	6055	C	TYR	D	108	69.018	75.966	183.473	1.00	42.87	D
ATOM	6056	O	TYR	D	108	70.147	75.886	182.997	1.00	40.59	D
ATOM	6057	N	LEU	D	109	68.356	77.109	183.595	1.00	43.90	D
ATOM	6058	CA	LEU	D	109	68.919	78.364	183.124	1.00	47.89	D
ATOM	6059	CB	LEU	D	109	67.960	78.981	182.102	1.00	45.04	D
ATOM	6060	CG	LEU	D	109	67.440	78.021	181.028	1.00	40.98	D
ATOM	6061	CD1	LEU	D	109	66.449	78.741	180.115	1.00	34.01	D
ATOM	6062	CD2	LEU	D	109	68.607	77.467	180.240	1.00	28.03	D
ATOM	6063	C	LEU	D	109	69.220	79.391	184.208	1.00	46.84	D
ATOM	6064	O	LEU	D	109	68.346	79.718	185.003	1.00	46.07	D
ATOM	6065	N	THR	D	110	70.455	79.901	184.213	1.00	46.09	D
ATOM	6066	CA	THR	D	110	70.894	80.907	185.179	1.00	44.66	D
ATOM	6067	CB	THR	D	110	72.131	80.447	185.954	1.00	46.31	D
ATOM	6068	OG1	THR	D	110	71.867	79.178	186.557	1.00	57.35	D
ATOM	6069	CG2	THR	D	110	72.466	81.446	187.051	1.00	49.15	D
ATOM	6070	C	THR	D	110	71.246	82.209	184.480	1.00	42.46	D
ATOM	6071	O	THR	D	110	72.117	82.248	183.597	1.00	40.46	D
ATOM	6072	N	PRO	D	111	70.578	83.302	184.872	1.00	41.92	D
ATOM	6073	CD	PRO	D	111	69.529	83.398	185.895	1.00	44.27	D
ATOM	6074	CA	PRO	D	111	70.826	84.613	184.269	1.00	44.00	D
ATOM	6075	CB	PRO	D	111	69.827	85.529	184.985	1.00	43.46	D
ATOM	6076	CG	PRO	D	111	68.750	84.606	185.427	1.00	45.40	D
ATOM	6077	C	PRO	D	111	72.255	85.056	184.496	1.00	42.86	D
ATOM	6078	O	PRO	D	111	72.867	84.709	185.511	1.00	40.66	D
ATOM	6079	N	VAL	D	112	72.782	85.814	183.542	1.00	42.41	D
ATOM	6080	CA	VAL	D	112	74.138	86.330	183.648	1.00	45.85	D
ATOM	6081	CB	VAL	D	112	74.788	86.531	182.260	1.00	46.02	D
ATOM	6082	CG1	VAL	D	112	75.008	85.173	181.598	1.00	41.03	D
ATOM	6083	CG2	VAL	D	112	73.907	87.438	181.394	1.00	34.23	D
ATOM	6084	C	VAL	D	112	74.069	87.664	184.364	1.00	49.28	D
ATOM	6085	O	VAL	D	112	73.026	88.320	184.369	1.00	51.96	D
ATOM	6086	N	SER	D	113	75.176	88.058	184.980	1.00	51.88	D
ATOM	6087	CA	SER	D	113	75.222	89.323	185.706	1.00	53.19	D
ATOM	6088	CB	SER	D	113	76.641	89.599	186.193	1.00	53.10	D
ATOM	6089	OG	SER	D	113	77.519	89.755	185.096	1.00	47.97	D
ATOM	6090	C	SER	D	113	74.760	90.492	184.844	1.00	53.57	D
ATOM	6091	O	SER	D	113	74.220	91.475	185.353	1.00	56.06	D
ATOM	6092	N	SER	D	114	74.968	90.384	183.537	1.00	51.32	D
ATOM	6093	CA	SER	D	114	74.584	91.454	182.634	1.00	51.91	D
ATOM	6094	CB	SER	D	114	75.488	91.434	181.399	1.00	53.07	D
ATOM	6095	OG	SER	D	114	75.306	90.260	180.641	1.00	54.30	D
ATOM	6096	C	SER	D	114	73.118	91.429	182.209	1.00	51.15	D
ATOM	6097	O	SER	D	114	72.658	92.311	181.495	1.00	51.08	D
ATOM	6098	N	ALA	D	115	72.380	90.429	182.666	1.00	53.13	D
ATOM	6099	CA	ALA	D	115	70.972	90.306	182.323	1.00	55.17	D



ATOM	6100	CB	ALA	D	115	70.392	89.074	182.999	1.00	59.33	D
ATOM	6101	C	ALA	D	115	70.163	91.548	182.712	1.00	56.57	D
ATOM	6102	O	ALA	D	115	70.132	91.937	183.886	1.00	53.06	D
ATOM	6103	N	GLY	D	116	69.490	92.143	181.720	1.00	58.70	D
ATOM	6104	CA	GLY	D	116	68.687	93.339	181.946	1.00	57.98	D
ATOM	6105	C	GLY	D	116	67.607	93.244	183.013	1.00	54.13	D
ATOM	6106	O	GLY	D	116	67.875	92.986	184.190	1.00	53.49	D
ATOM	6107	N	GLY	D	117	66.378	93.504	182.597	1.00	51.13	D
ATOM	6108	CA	GLY	D	117	65.247	93.419	183.502	1.00	49.54	D
ATOM	6109	C	GLY	D	117	64.444	92.257	182.953	1.00	45.32	D
ATOM	6110	O	GLY	D	117	64.316	91.219	183.601	1.00	41.28	D
ATOM	6111	N	VAL	D	118	63.926	92.442	181.738	1.00	43.53	D
ATOM	6112	CA	VAL	D	118	63.172	91.418	181.025	1.00	39.62	D
ATOM	6113	CB	VAL	D	118	62.195	92.048	180.049	1.00	36.60	D
ATOM	6114	CG1	VAL	D	118	61.689	91.006	179.068	1.00	33.90	D
ATOM	6115	CG2	VAL	D	118	61.049	92.667	180.825	1.00	37.97	D
ATOM	6116	C	VAL	D	118	64.158	90.581	180.225	1.00	36.77	D
ATOM	6117	O	VAL	D	118	64.528	90.966	179.139	1.00	40.52	D
ATOM	6118	N	ALA	D	119	64.585	89.443	180.760	1.00	33.72	D
ATOM	6119	CA	ALA	D	119	65.538	88.595	180.063	1.00	32.65	D
ATOM	6120	CB	ALA	D	119	66.347	87.804	181.068	1.00	30.48	D
ATOM	6121	C	ALA	D	119	64.896	87.641	179.051	1.00	35.66	D
ATOM	6122	O	ALA	D	119	65.601	87.014	178.264	1.00	34.93	D
ATOM	6123	N	ILE	D	120	63.571	87.513	179.098	1.00	35.52	D
ATOM	6124	CA	ILE	D	120	62.824	86.658	178.179	1.00	34.90	D
ATOM	6125	CB	ILE	D	120	62.596	85.264	178.771	1.00	38.09	D
ATOM	6126	CG2	ILE	D	120	61.650	84.470	177.887	1.00	30.29	D
ATOM	6127	CG1	ILE	D	120	63.921	84.527	178.911	1.00	38.37	D
ATOM	6128	CD1	ILE	D	120	63.783	83.171	179.571	1.00	36.87	D
ATOM	6129	C	ILE	D	120	61.449	87.280	177.900	1.00	37.61	D
ATOM	6130	O	ILE	D	120	60.647	87.462	178.818	1.00	41.13	D
ATOM	6131	N	LYS	D	121	61.168	87.600	176.643	1.00	32.47	D
ATOM	6132	CA	LYS	D	121	59.880	88.193	176.321	1.00	36.26	D
ATOM	6133	CB	LYS	D	121	59.930	88.923	174.968	1.00	46.31	D
ATOM	6134	CG	LYS	D	121	60.415	90.375	174.977	1.00	49.15	D
ATOM	6135	CD	LYS	D	121	61.887	90.475	175.358	1.00	62.54	D
ATOM	6136	CE	LYS	D	121	62.463	91.829	174.973	1.00	65.40	D
ATOM	6137	NZ	LYS	D	121	62.286	92.089	173.509	1.00	67.14	D
ATOM	6138	C	LYS	D	121	58.693	87.227	176.291	1.00	35.22	D
ATOM	6139	O	LYS	D	121	58.786	86.070	175.864	1.00	33.57	D
ATOM	6140	N	ALA	D	122	57.564	87.732	176.758	1.00	33.71	D
ATOM	6141	CA	ALA	D	122	56.339	86.971	176.736	1.00	33.24	D
ATOM	6142	CB	ALA	D	122	55.205	87.794	177.364	1.00	19.80	D
ATOM	6143	C	ALA	D	122	56.042	86.691	175.250	1.00	34.23	D
ATOM	6144	O	ALA	D	122	56.067	87.606	174.413	1.00	35.03	D
ATOM	6145	N	GLY	D	123	55.783	85.428	174.930	1.00	32.35	D
ATOM	6146	CA	GLY	D	123	55.464	85.053	173.564	1.00	31.57	D
ATOM	6147	C	GLY	D	123	56.649	84.707	172.682	1.00	31.64	D
ATOM	6148	O	GLY	D	123	56.478	84.377	171.515	1.00	33.03	D
ATOM	6149	N	SER	D	124	57.854	84.750	173.229	1.00	30.96	D
ATOM	6150	CA	SER	D	124	59.031	84.474	172.422	1.00	31.06	D
ATOM	6151	CB	SER	D	124	60.210	85.334	172.918	1.00	31.98	D
ATOM	6152	OG	SER	D	124	60.508	85.135	174.290	1.00	21.85	D
ATOM	6153	C	SER	D	124	59.479	83.019	172.296	1.00	32.52	D
ATOM	6154	O	SER	D	124	59.207	82.169	173.147	1.00	31.79	D
ATOM	6155	N	LEU	D	125	60.187	82.740	171.213	1.00	31.44	D
ATOM	6156	CA	LEU	D	125	60.692	81.402	171.005	1.00	31.36	D
ATOM	6157	CB	LEU	D	125	61.200	81.196	169.573	1.00	29.94	D



ATOM	6158	CG	LEU	D	125	61.949	79.870	169.410	1.00	28.69	D
ATOM	6159	CD1	LEU	D	125	60.979	78.717	169.659	1.00	15.55	D
ATOM	6160	CD2	LEU	D	125	62.569	79.778	168.036	1.00	22.97	D
ATOM	6161	C	LEU	D	125	61.841	81.361	171.957	1.00	28.90	D
ATOM	6162	O	LEU	D	125	62.789	82.119	171.833	1.00	31.79	D
ATOM	6163	N	ILE	D	126	61.749	80.467	172.914	1.00	32.84	D
ATOM	6164	CA	ILE	D	126	62.771	80.338	173.933	1.00	33.09	D
ATOM	6165	CB	ILE	D	126	62.081	80.159	175.298	1.00	35.71	D
ATOM	6166	CG2	ILE	D	126	62.463	78.847	175.962	1.00	23.65	D
ATOM	6167	CG1	ILE	D	126	62.341	81.391	176.127	1.00	30.61	D
ATOM	6168	CD1	ILE	D	126	61.580	81.367	177.402	1.00	53.93	D
ATOM	6169	C	ILE	D	126	63.726	79.209	173.634	1.00	33.05	D
ATOM	6170	O	ILE	D	126	64.889	79.307	173.968	1.00	31.46	D
ATOM	6171	N	ALA	D	127	63.237	78.147	172.989	1.00	32.78	D
ATOM	6172	CA	ALA	D	127	64.079	76.995	172.657	1.00	29.06	D
ATOM	6173	CB	ALA	D	127	64.422	76.232	173.918	1.00	25.72	D
ATOM	6174	C	ALA	D	127	63.450	76.031	171.652	1.00	27.75	D
ATOM	6175	O	ALA	D	127	62.229	75.977	171.498	1.00	30.67	D
ATOM	6176	N	VAL	D	128	64.298	75.283	170.959	1.00	20.04	D
ATOM	6177	CA	VAL	D	128	63.828	74.288	170.021	1.00	21.96	D
ATOM	6178	CB	VAL	D	128	64.206	74.629	168.564	1.00	21.52	D
ATOM	6179	CG1	VAL	D	128	63.886	73.437	167.659	1.00	17.02	D
ATOM	6180	CG2	VAL	D	128	63.418	75.841	168.086	1.00	20.28	D
ATOM	6181	C	VAL	D	128	64.505	72.979	170.421	1.00	26.34	D
ATOM	6182	O	VAL	D	128	65.734	72.906	170.435	1.00	28.68	D
ATOM	6183	N	LEU	D	129	63.710	71.960	170.757	1.00	24.52	D
ATOM	6184	CA	LEU	D	129	64.254	70.670	171.169	1.00	26.06	D
ATOM	6185	CB	LEU	D	129	63.726	70.291	172.548	1.00	26.54	D
ATOM	6186	CG	LEU	D	129	64.049	71.260	173.685	1.00	33.57	D
ATOM	6187	CD1	LEU	D	129	63.480	70.722	174.970	1.00	18.74	D
ATOM	6188	CD2	LEU	D	129	65.565	71.438	173.813	1.00	34.02	D
ATOM	6189	C	LEU	D	129	63.910	69.562	170.183	1.00	30.38	D
ATOM	6190	O	LEU	D	129	62.734	69.333	169.860	1.00	31.27	D
ATOM	6191	N	ILE	D	130	64.940	68.862	169.714	1.00	26.82	D
ATOM	6192	CA	ILE	D	130	64.725	67.788	168.761	1.00	28.16	D
ATOM	6193	CB	ILE	D	130	65.699	67.876	167.566	1.00	29.84	D
ATOM	6194	CG2	ILE	D	130	65.502	66.687	166.632	1.00	24.68	D
ATOM	6195	CG1	ILE	D	130	65.424	69.157	166.779	1.00	26.91	D
ATOM	6196	CD1	ILE	D	130	66.417	69.391	165.682	1.00	35.59	D
ATOM	6197	C	ILE	D	130	64.842	66.414	169.382	1.00	31.09	D
ATOM	6198	O	ILE	D	130	65.910	66.002	169.858	1.00	30.21	D
ATOM	6199	N	LEU	D	131	63.710	65.719	169.356	1.00	33.55	D
ATOM	6200	CA	LEU	D	131	63.575	64.379	169.876	1.00	31.28	D
ATOM	6201	CB	LEU	D	131	62.174	64.211	170.454	1.00	29.44	D
ATOM	6202	CG	LEU	D	131	61.878	62.859	171.089	1.00	35.20	D
ATOM	6203	CD1	LEU	D	131	60.662	62.990	171.994	1.00	34.24	D
ATOM	6204	CD2	LEU	D	131	61.670	61.810	170.002	1.00	34.36	D
ATOM	6205	C	LEU	D	131	63.787	63.437	168.702	1.00	30.98	D
ATOM	6206	O	LEU	D	131	63.101	63.544	167.699	1.00	30.92	D
ATOM	6207	N	ARG	D	132	64.743	62.519	168.833	1.00	34.57	D
ATOM	6208	CA	ARG	D	132	65.042	61.548	167.778	1.00	34.76	D
ATOM	6209	CB	ARG	D	132	66.511	61.620	167.409	1.00	31.73	D
ATOM	6210	CG	ARG	D	132	66.934	60.634	166.377	1.00	25.08	D
ATOM	6211	CD	ARG	D	132	68.340	60.935	166.004	1.00	30.94	D
ATOM	6212	NE	ARG	D	132	68.698	60.392	164.702	1.00	48.14	D
ATOM	6213	CZ	ARG	D	132	69.821	60.702	164.059	1.00	54.00	D
ATOM	6214	NH1	ARG	D	132	70.689	61.552	164.605	1.00	54.78	D
ATOM	6215	NH2	ARG	D	132	70.078	60.173	162.866	1.00	55.96	D



ATOM	6216	C	ARG	D	132	64.700	60.139	168.244	1.00	38.33	D
ATOM	6217	O	ARG	D	132	65.256	59.648	169.230	1.00	38.52	D
ATOM	6218	N	GLN	D	133	63.792	59.494	167.513	1.00	38.39	D
ATOM	6219	CA	GLN	D	133	63.317	58.158	167.850	1.00	33.51	D
ATOM	6220	CB	GLN	D	133	61.819	58.212	168.123	1.00	30.61	D
ATOM	6221	CG	GLN	D	133	61.149	56.859	168.321	1.00	39.48	D
ATOM	6222	CD	GLN	D	133	60.552	56.280	167.045	1.00	36.71	D
ATOM	6223	OE1	GLN	D	133	59.736	56.910	166.382	1.00	41.51	D
ATOM	6224	NE2	GLN	D	133	60.955	55.069	166.708	1.00	35.25	D
ATOM	6225	C	GLN	D	133	63.600	57.110	166.796	1.00	34.18	D
ATOM	6226	O	GLN	D	133	63.279	57.281	165.620	1.00	36.28	D
ATOM	6227	N	THR	D	134	64.215	56.023	167.241	1.00	33.02	D
ATOM	6228	CA	THR	D	134	64.547	54.876	166.398	1.00	32.17	D
ATOM	6229	CB	THR	D	134	66.044	54.702	166.287	1.00	30.15	D
ATOM	6230	OG1	THR	D	134	66.609	54.883	167.593	1.00	44.11	D
ATOM	6231	CG2	THR	D	134	66.634	55.692	165.317	1.00	22.68	D
ATOM	6232	C	THR	D	134	63.982	53.630	167.101	1.00	35.50	D
ATOM	6233	O	THR	D	134	63.174	53.739	168.037	1.00	32.36	D
ATOM	6234	N	ASN	D	135	64.404	52.445	166.669	1.00	35.58	D
ATOM	6235	CA	ASN	D	135	63.902	51.237	167.304	1.00	41.05	D
ATOM	6236	CB	ASN	D	135	62.469	50.964	166.859	1.00	40.87	D
ATOM	6237	CG	ASN	D	135	62.345	50.879	165.360	1.00	41.94	D
ATOM	6238	OD1	ASN	D	135	63.211	50.322	164.689	1.00	43.65	D
ATOM	6239	ND2	ASN	D	135	61.266	51.429	164.823	1.00	41.79	D
ATOM	6240	C	ASN	D	135	64.754	50.029	166.993	1.00	43.39	D
ATOM	6241	O	ASN	D	135	65.665	50.093	166.163	1.00	43.85	D
ATOM	6242	N	ASN	D	136	64.449	48.927	167.669	1.00	44.82	D
ATOM	6243	CA	ASN	D	136	65.166	47.679	167.450	1.00	49.97	D
ATOM	6244	CB	ASN	D	136	65.318	46.917	168.753	1.00	49.65	D
ATOM	6245	CG	ASN	D	136	63.987	46.597	169.388	1.00	55.20	D
ATOM	6246	OD1	ASN	D	136	63.924	46.031	170.481	1.00	58.92	D
ATOM	6247	ND2	ASN	D	136	62.907	46.963	168.709	1.00	55.27	D
ATOM	6248	C	ASN	D	136	64.371	46.827	166.481	1.00	53.16	D
ATOM	6249	O	ASN	D	136	64.345	45.602	166.601	1.00	53.71	D
ATOM	6250	N	TYR	D	137	63.704	47.481	165.534	1.00	55.41	D
ATOM	6251	CA	TYR	D	137	62.903	46.757	164.566	1.00	55.16	D
ATOM	6252	CB	TYR	D	137	61.416	47.039	164.769	1.00	60.51	D
ATOM	6253	CG	TYR	D	137	60.548	46.240	163.824	1.00	71.04	D
ATOM	6254	CD1	TYR	D	137	60.646	44.846	163.763	1.00	68.96	D
ATOM	6255	CE1	TYR	D	137	59.861	44.108	162.880	1.00	72.76	D
ATOM	6256	CD2	TYR	D	137	59.637	46.876	162.972	1.00	75.48	D
ATOM	6257	CE2	TYR	D	137	58.845	46.142	162.084	1.00	74.32	D
ATOM	6258	CZ	TYR	D	137	58.964	44.763	162.046	1.00	73.15	D
ATOM	6259	OH	TYR	D	137	58.184	44.043	161.179	1.00	72.59	D
ATOM	6260	C	TYR	D	137	63.266	47.023	163.123	1.00	52.42	D
ATOM	6261	O	TYR	D	137	63.283	46.094	162.329	1.00	54.24	D
ATOM	6262	N	ASN	D	138	63.553	48.275	162.776	1.00	49.30	D
ATOM	6263	CA	ASN	D	138	63.916	48.603	161.399	1.00	49.09	D
ATOM	6264	CB	ASN	D	138	62.667	48.719	160.540	1.00	48.86	D
ATOM	6265	CG	ASN	D	138	61.705	49.752	161.051	1.00	44.77	D
ATOM	6266	OD1	ASN	D	138	60.623	49.894	160.517	1.00	46.88	D
ATOM	6267	ND2	ASN	D	138	62.095	50.486	162.084	1.00	44.57	D
ATOM	6268	C	ASN	D	138	64.727	49.882	161.279	1.00	52.13	D
ATOM	6269	O	ASN	D	138	65.282	50.360	162.268	1.00	54.23	D
ATOM	6270	N	SER	D	139	64.790	50.442	160.071	1.00	52.55	D
ATOM	6271	CA	SER	D	139	65.564	51.665	159.857	1.00	52.05	D
ATOM	6272	CB	SER	D	139	66.094	51.709	158.418	1.00	54.53	D
ATOM	6273	OG	SER	D	139	65.031	51.753	157.480	1.00	64.83	D



ATOM	6274	C	SER	D	139	64.828	52.974	160.170	1.00	45.51	D
ATOM	6275	O	SER	D	139	65.229	54.038	159.699	1.00	41.72	D
ATOM	6276	N	ASP	D	140	63.763	52.895	160.965	1.00	43.15	D
ATOM	6277	CA	ASP	D	140	63.003	54.086	161.340	1.00	44.07	D
ATOM	6278	CB	ASP	D	140	61.744	53.694	162.129	1.00	42.00	D
ATOM	6279	CG	ASP	D	140	60.593	53.266	161.228	1.00	44.72	D
ATOM	6280	OD1	ASP	D	140	59.534	52.848	161.755	1.00	39.06	D
ATOM	6281	OD2	ASP	D	140	60.743	53.350	159.987	1.00	44.25	D
ATOM	6282	C	ASP	D	140	63.843	55.077	162.163	1.00	44.58	D
ATOM	6283	O	ASP	D	140	64.341	54.757	163.241	1.00	40.77	D
ATOM	6284	N	ASP	D	141	63.990	56.286	161.639	1.00	46.87	D
ATOM	6285	CA	ASP	D	141	64.747	57.345	162.302	1.00	44.40	D
ATOM	6286	CB	ASP	D	141	66.113	57.487	161.636	1.00	48.13	D
ATOM	6287	CG	ASP	D	141	67.092	58.291	162.464	1.00	54.26	D
ATOM	6288	OD1	ASP	D	141	66.660	59.093	163.322	1.00	56.40	D
ATOM	6289	OD2	ASP	D	141	68.307	58.126	162.235	1.00	58.45	D
ATOM	6290	C	ASP	D	141	63.930	58.628	162.103	1.00	41.56	D
ATOM	6291	O	ASP	D	141	64.118	59.342	161.116	1.00	42.25	D
ATOM	6292	N	PHE	D	142	63.022	58.906	163.031	1.00	34.64	D
ATOM	6293	CA	PHE	D	142	62.154	60.074	162.930	1.00	35.62	D
ATOM	6294	CB	PHE	D	142	60.691	59.659	163.148	1.00	32.21	D
ATOM	6295	CG	PHE	D	142	60.208	58.613	162.189	1.00	36.37	D
ATOM	6296	CD1	PHE	D	142	59.562	57.468	162.659	1.00	40.98	D
ATOM	6297	CD2	PHE	D	142	60.361	58.777	160.812	1.00	28.49	D
ATOM	6298	CE1	PHE	D	142	59.065	56.503	161.769	1.00	34.40	D
ATOM	6299	CE2	PHE	D	142	59.873	57.829	159.927	1.00	30.18	D
ATOM	6300	CZ	PHE	D	142	59.221	56.688	160.408	1.00	32.89	D
ATOM	6301	C	PHE	D	142	62.508	61.172	163.921	1.00	37.65	D
ATOM	6302	O	PHE	D	142	63.052	60.915	165.000	1.00	39.93	D
ATOM	6303	N	GLN	D	143	62.178	62.405	163.559	1.00	35.40	D
ATOM	6304	CA	GLN	D	143	62.467	63.531	164.426	1.00	30.59	D
ATOM	6305	CB	GLN	D	143	63.374	64.531	163.726	1.00	26.22	D
ATOM	6306	CG	GLN	D	143	64.757	64.051	163.426	1.00	31.74	D
ATOM	6307	CD	GLN	D	143	65.664	65.204	163.100	1.00	44.27	D
ATOM	6308	OE1	GLN	D	143	65.267	66.123	162.384	1.00	45.79	D
ATOM	6309	NE2	GLN	D	143	66.892	65.176	163.626	1.00	52.76	D
ATOM	6310	C	GLN	D	143	61.204	64.244	164.848	1.00	30.08	D
ATOM	6311	O	GLN	D	143	60.353	64.562	164.025	1.00	30.98	D
ATOM	6312	N	PHE	D	144	61.093	64.484	166.145	1.00	30.40	D
ATOM	6313	CA	PHE	D	144	59.953	65.176	166.706	1.00	28.23	D
ATOM	6314	CB	PHE	D	144	59.343	64.366	167.841	1.00	27.48	D
ATOM	6315	CG	PHE	D	144	58.663	63.113	167.379	1.00	27.17	D
ATOM	6316	CD1	PHE	D	144	59.398	62.061	166.845	1.00	27.61	D
ATOM	6317	CD2	PHE	D	144	57.278	62.981	167.476	1.00	28.73	D
ATOM	6318	CE1	PHE	D	144	58.759	60.885	166.414	1.00	23.50	D
ATOM	6319	CE2	PHE	D	144	56.633	61.817	167.051	1.00	21.46	D
ATOM	6320	CZ	PHE	D	144	57.379	60.768	166.521	1.00	19.26	D
ATOM	6321	C	PHE	D	144	60.495	66.487	167.209	1.00	28.85	D
ATOM	6322	O	PHE	D	144	61.233	66.516	168.194	1.00	31.92	D
ATOM	6323	N	VAL	D	145	60.123	67.570	166.527	1.00	23.53	D
ATOM	6324	CA	VAL	D	145	60.608	68.880	166.878	1.00	21.18	D
ATOM	6325	CB	VAL	D	145	60.867	69.693	165.609	1.00	23.24	D
ATOM	6326	CG1	VAL	D	145	61.379	71.061	165.972	1.00	18.08	D
ATOM	6327	CG2	VAL	D	145	61.889	68.965	164.719	1.00	18.41	D
ATOM	6328	C	VAL	D	145	59.692	69.649	167.789	1.00	26.00	D
ATOM	6329	O	VAL	D	145	58.523	69.850	167.475	1.00	33.86	D
ATOM	6330	N	TRP	D	146	60.222	70.085	168.928	1.00	27.40	D
ATOM	6331	CA	TRP	D	146	59.424	70.853	169.882	1.00	26.75	D



ATOM	6332	CB	TRP	D	146	59.506	70.212	171.275	1.00	25.43	D
ATOM	6333	CG	TRP	D	146	59.261	68.728	171.236	1.00	27.11	D
ATOM	6334	CD2	TRP	D	146	57.992	68.065	171.210	1.00	23.03	D
ATOM	6335	CE2	TRP	D	146	58.246	66.681	171.078	1.00	26.00	D
ATOM	6336	CE3	TRP	D	146	56.663	68.505	171.278	1.00	24.17	D
ATOM	6337	CD1	TRP	D	146	60.205	67.747	171.124	1.00	27.33	D
ATOM	6338	NE1	TRP	D	146	59.605	66.515	171.025	1.00	30.19	D
ATOM	6339	CZ2	TRP	D	146	57.217	65.730	171.022	1.00	24.41	D
ATOM	6340	CZ3	TRP	D	146	55.629	67.547	171.217	1.00	22.87	D
ATOM	6341	CH2	TRP	D	146	55.919	66.182	171.092	1.00	16.39	D
ATOM	6342	C	TRP	D	146	59.878	72.313	169.925	1.00	28.37	D
ATOM	6343	O	TRP	D	146	61.049	72.619	170.175	1.00	28.62	D
ATOM	6344	N	ASN	D	147	58.951	73.219	169.642	1.00	27.25	D
ATOM	6345	CA	ASN	D	147	59.271	74.638	169.667	1.00	26.16	D
ATOM	6346	CB	ASN	D	147	58.650	75.354	168.456	1.00	23.89	D
ATOM	6347	CG	ASN	D	147	59.114	74.766	167.134	1.00	27.09	D
ATOM	6348	OD1	ASN	D	147	60.314	74.571	166.898	1.00	20.08	D
ATOM	6349	ND2	ASN	D	147	58.167	74.486	166.263	1.00	29.99	D
ATOM	6350	C	ASN	D	147	58.729	75.192	170.969	1.00	26.56	D
ATOM	6351	O	ASN	D	147	57.512	75.309	171.140	1.00	27.81	D
ATOM	6352	N	ILE	D	148	59.639	75.522	171.884	1.00	24.13	D
ATOM	6353	CA	ILE	D	148	59.260	76.033	173.197	1.00	25.61	D
ATOM	6354	CB	ILE	D	148	60.325	75.660	174.261	1.00	27.27	D
ATOM	6355	CG2	ILE	D	148	59.691	75.697	175.646	1.00	27.75	D
ATOM	6356	CG1	ILE	D	148	60.980	74.299	173.935	1.00	29.39	D
ATOM	6357	CD1	ILE	D	148	60.068	73.070	173.920	1.00	17.68	D
ATOM	6358	C	ILE	D	148	59.072	77.546	173.264	1.00	24.39	D
ATOM	6359	O	ILE	D	148	60.029	78.293	173.129	1.00	31.25	D
ATOM	6360	N	TYR	D	149	57.849	77.999	173.479	1.00	21.31	D
ATOM	6361	CA	TYR	D	149	57.577	79.427	173.608	1.00	26.14	D
ATOM	6362	CB	TYR	D	149	56.372	79.834	172.753	1.00	22.48	D
ATOM	6363	CG	TYR	D	149	56.648	79.869	171.275	1.00	26.88	D
ATOM	6364	CD1	TYR	D	149	56.710	78.689	170.523	1.00	28.49	D
ATOM	6365	CE1	TYR	D	149	56.985	78.718	169.166	1.00	27.20	D
ATOM	6366	CD2	TYR	D	149	56.870	81.080	170.623	1.00	30.75	D
ATOM	6367	CE2	TYR	D	149	57.150	81.122	169.261	1.00	29.69	D
ATOM	6368	CZ	TYR	D	149	57.204	79.942	168.538	1.00	31.37	D
ATOM	6369	OH	TYR	D	149	57.469	79.987	167.190	1.00	32.39	D
ATOM	6370	C	TYR	D	149	57.279	79.783	175.076	1.00	30.05	D
ATOM	6371	O	TYR	D	149	56.691	78.981	175.800	1.00	34.32	D
ATOM	6372	N	ALA	D	150	57.687	80.974	175.514	1.00	31.39	D
ATOM	6373	CA	ALA	D	150	57.420	81.418	176.880	1.00	30.53	D
ATOM	6374	CB	ALA	D	150	58.557	82.214	177.398	1.00	25.01	D
ATOM	6375	C	ALA	D	150	56.160	82.267	176.847	1.00	32.63	D
ATOM	6376	O	ALA	D	150	56.033	83.149	176.011	1.00	37.10	D
ATOM	6377	N	ASN	D	151	55.230	82.002	177.755	1.00	30.51	D
ATOM	6378	CA	ASN	D	151	53.975	82.732	177.773	1.00	31.76	D
ATOM	6379	CB	ASN	D	151	52.896	81.929	178.500	1.00	37.84	D
ATOM	6380	CG	ASN	D	151	52.346	80.792	177.671	1.00	41.40	D
ATOM	6381	OD1	ASN	D	151	51.861	80.997	176.557	1.00	42.29	D
ATOM	6382	ND2	ASN	D	151	52.413	79.583	178.213	1.00	39.30	D
ATOM	6383	C	ASN	D	151	54.076	84.069	178.446	1.00	32.29	D
ATOM	6384	O	ASN	D	151	53.235	84.941	178.238	1.00	36.96	D
ATOM	6385	N	ASN	D	152	55.111	84.235	179.253	1.00	31.47	D
ATOM	6386	CA	ASN	D	152	55.271	85.459	180.014	1.00	30.73	D
ATOM	6387	CB	ASN	D	152	54.772	85.211	181.421	1.00	29.45	D
ATOM	6388	CG	ASN	D	152	55.627	84.195	182.155	1.00	33.46	D
ATOM	6389	OD1	ASN	D	152	55.540	82.991	181.906	1.00	42.29	D



ATOM	6390	ND2	ASN	D	152	56.478	84.679	183.050	1.00	34.86	D
ATOM	6391	C	ASN	D	152	56.710	85.944	180.102	1.00	32.32	D
ATOM	6392	O	ASN	D	152	57.652	85.201	179.777	1.00	22.60	D
ATOM	6393	N	ASP	D	153	56.868	87.185	180.576	1.00	32.96	D
ATOM	6394	CA	ASP	D	153	58.199	87.758	180.733	1.00	34.17	D
ATOM	6395	CB	ASP	D	153	58.175	89.275	180.989	1.00	33.81	D
ATOM	6396	CG	ASP	D	153	57.575	90.087	179.852	1.00	41.74	D
ATOM	6397	OD1	ASP	D	153	57.581	89.650	178.674	1.00	43.26	D
ATOM	6398	OD2	ASP	D	153	57.116	91.206	180.162	1.00	36.22	D
ATOM	6399	C	ASP	D	153	58.869	87.150	181.951	1.00	33.17	D
ATOM	6400	O	ASP	D	153	58.223	86.915	182.966	1.00	33.49	D
ATOM	6401	N	VAL	D	154	60.162	86.891	181.833	1.00	30.92	D
ATOM	6402	CA	VAL	D	154	60.959	86.421	182.943	1.00	31.38	D
ATOM	6403	CB	VAL	D	154	61.767	85.188	182.585	1.00	33.39	D
ATOM	6404	CG1	VAL	D	154	62.727	84.833	183.738	1.00	29.51	D
ATOM	6405	CG2	VAL	D	154	60.843	84.060	182.308	1.00	37.67	D
ATOM	6406	C	VAL	D	154	61.939	87.572	183.261	1.00	33.41	D
ATOM	6407	O	VAL	D	154	62.927	87.798	182.550	1.00	30.75	D
ATOM	6408	N	VAL	D	155	61.639	88.309	184.321	1.00	34.81	D
ATOM	6409	CA	VAL	D	155	62.469	89.429	184.754	1.00	34.30	D
ATOM	6410	CB	VAL	D	155	61.635	90.516	185.516	1.00	33.55	D
ATOM	6411	CG1	VAL	D	155	62.560	91.436	186.289	1.00	37.26	D
ATOM	6412	CG2	VAL	D	155	60.807	91.337	184.536	1.00	38.10	D
ATOM	6413	C	VAL	D	155	63.586	88.996	185.689	1.00	32.23	D
ATOM	6414	O	VAL	D	155	63.384	88.172	186.581	1.00	29.51	D
ATOM	6415	N	VAL	D	156	64.766	89.563	185.468	1.00	35.10	D
ATOM	6416	CA	VAL	D	156	65.929	89.321	186.321	1.00	38.71	D
ATOM	6417	CB	VAL	D	156	67.150	88.920	185.513	1.00	42.06	D
ATOM	6418	CG1	VAL	D	156	68.394	89.027	186.388	1.00	36.41	D
ATOM	6419	CG2	VAL	D	156	66.962	87.497	184.970	1.00	41.89	D
ATOM	6420	C	VAL	D	156	66.220	90.665	186.980	1.00	38.78	D
ATOM	6421	O	VAL	D	156	66.744	91.570	186.334	1.00	41.23	D
ATOM	6422	N	PRO	D	157	65.890	90.813	188.274	1.00	38.55	D
ATOM	6423	CD	PRO	D	157	65.442	89.754	189.189	1.00	37.36	D
ATOM	6424	CA	PRO	D	157	66.109	92.064	189.014	1.00	38.18	D
ATOM	6425	CB	PRO	D	157	65.747	91.689	190.444	1.00	37.79	D
ATOM	6426	CG	PRO	D	157	64.770	90.555	190.262	1.00	38.73	D
ATOM	6427	C	PRO	D	157	67.527	92.605	188.912	1.00	36.55	D
ATOM	6428	O	PRO	D	157	68.503	91.836	188.876	1.00	36.02	D
ATOM	6429	N	THR	D	158	67.638	93.928	188.839	1.00	32.19	D
ATOM	6430	CA	THR	D	158	68.953	94.542	188.767	1.00	37.42	D
ATOM	6431	CB	THR	D	158	68.867	95.995	188.317	1.00	41.41	D
ATOM	6432	OG1	THR	D	158	70.150	96.610	188.479	1.00	46.90	D
ATOM	6433	CG2	THR	D	158	67.862	96.741	189.143	1.00	46.90	D
ATOM	6434	C	THR	D	158	69.621	94.484	190.147	1.00	36.73	D
ATOM	6435	O	THR	D	158	68.974	94.742	191.167	1.00	34.96	D
ATOM	6436	N	GLY	D	159	70.906	94.124	190.171	1.00	35.62	D
ATOM	6437	CA	GLY	D	159	71.643	94.028	191.426	1.00	36.28	D
ATOM	6438	C	GLY	D	159	72.313	95.316	191.907	1.00	37.83	D
ATOM	6439	O	GLY	D	159	72.196	96.379	191.276	1.00	35.38	D
ATOM	6440	N	GLY	D	160	73.000	95.237	193.043	1.00	35.09	D
ATOM	6441	CA	GLY	D	160	73.672	96.418	193.547	1.00	36.59	D
ATOM	6442	C	GLY	D	160	75.037	96.477	192.903	1.00	37.35	D
ATOM	6443	O	GLY	D	160	75.482	95.471	192.353	1.00	38.20	D
ATOM	6444	N	CYS	D	161	75.709	97.625	192.962	1.00	37.82	D
ATOM	6445	CA	CYS	D	161	77.035	97.746	192.361	1.00	40.12	D
ATOM	6446	C	CYS	D	161	78.174	97.290	193.287	1.00	41.94	D
ATOM	6447	O	CYS	D	161	77.955	96.998	194.466	1.00	44.24	D



ATOM	6448	CB	CYS	D	161	77.249	99.177	191.933	1.00	41.37	D
ATOM	6449	SG	CYS	D	161	75.851	99.818	190.963	1.00	45.93	D
ATOM	6450	N	ASP	D	162	79.386	97.187	192.751	1.00	42.14	D
ATOM	6451	CA	ASP	D	162	80.504	96.765	193.581	1.00	46.77	D
ATOM	6452	CB	ASP	D	162	81.269	95.599	192.961	1.00	51.85	D
ATOM	6453	CG	ASP	D	162	82.246	94.956	193.949	1.00	64.21	D
ATOM	6454	OD1	ASP	D	162	81.835	94.651	195.095	1.00	64.19	D
ATOM	6455	OD2	ASP	D	162	83.425	94.750	193.584	1.00	70.74	D
ATOM	6456	C	ASP	D	162	81.438	97.930	193.801	1.00	50.77	D
ATOM	6457	O	ASP	D	162	81.841	98.618	192.860	1.00	52.21	D
ATOM	6458	N	VAL	D	163	81.765	98.157	195.063	1.00	51.82	D
ATOM	6459	CA	VAL	D	163	82.627	99.253	195.430	1.00	56.60	D
ATOM	6460	CB	VAL	D	163	82.082	99.959	196.671	1.00	54.71	D
ATOM	6461	CG1	VAL	D	163	83.012	101.072	197.094	1.00	56.74	D
ATOM	6462	CG2	VAL	D	163	80.688	100.512	196.367	1.00	51.81	D
ATOM	6463	C	VAL	D	163	84.030	98.741	195.666	1.00	64.32	D
ATOM	6464	O	VAL	D	163	84.436	98.455	196.787	1.00	65.70	D
ATOM	6465	N	SER	D	164	84.763	98.628	194.569	1.00	74.12	D
ATOM	6466	CA	SER	D	164	86.134	98.150	194.573	1.00	81.28	D
ATOM	6467	CB	SER	D	164	86.643	98.068	193.128	1.00	83.04	D
ATOM	6468	OG	SER	D	164	85.623	97.607	192.250	1.00	74.81	D
ATOM	6469	C	SER	D	164	87.020	99.094	195.383	1.00	86.27	D
ATOM	6470	O	SER	D	164	87.278	100.232	194.963	1.00	86.58	D
ATOM	6471	N	ALA	D	165	87.475	98.615	196.541	1.00	90.59	D
ATOM	6472	CA	ALA	D	165	88.348	99.391	197.426	1.00	95.36	D
ATOM	6473	CB	ALA	D	165	87.565	99.866	198.648	1.00	94.09	D
ATOM	6474	C	ALA	D	165	89.539	98.532	197.864	1.00	98.36	D
ATOM	6475	O	ALA	D	165	89.364	97.378	198.267	1.00	101.61	D
ATOM	6476	N	ARG	D	166	90.746	99.089	197.784	1.00	98.81	D
ATOM	6477	CA	ARG	D	166	91.944	98.351	198.170	1.00	99.39	D
ATOM	6478	CB	ARG	D	166	93.181	99.203	197.894	1.00	97.36	D
ATOM	6479	CG	ARG	D	166	93.276	99.594	196.426	1.00	95.00	D
ATOM	6480	CD	ARG	D	166	94.549	100.351	196.083	1.00	96.49	D
ATOM	6481	NE	ARG	D	166	94.568	100.744	194.671	1.00	96.19	D
ATOM	6482	CZ	ARG	D	166	95.473	101.551	194.120	1.00	94.46	D
ATOM	6483	NH1	ARG	D	166	96.451	102.062	194.859	1.00	91.13	D
ATOM	6484	NH2	ARG	D	166	95.392	101.857	192.830	1.00	93.77	D
ATOM	6485	C	ARG	D	166	91.888	97.883	199.629	1.00	101.99	D
ATOM	6486	O	ARG	D	166	91.831	96.672	199.869	1.00	104.31	D
ATOM	6487	N	ASP	D	167	91.902	98.817	200.589	1.00	101.69	D
ATOM	6488	CA	ASP	D	167	91.805	98.483	202.027	1.00	101.34	D
ATOM	6489	CB	ASP	D	167	92.798	97.381	202.426	1.00	104.24	D
ATOM	6490	CG	ASP	D	167	92.590	96.890	203.868	1.00	107.74	D
ATOM	6491	OD1	ASP	D	167	93.471	96.171	204.390	1.00	111.70	D
ATOM	6492	OD2	ASP	D	167	91.547	97.218	204.483	1.00	105.67	D
ATOM	6493	C	ASP	D	167	92.012	99.671	202.967	1.00	99.65	D
ATOM	6494	O	ASP	D	167	91.759	100.818	202.599	1.00	101.50	D
ATOM	6495	N	VAL	D	168	92.461	99.366	204.187	1.00	95.26	D
ATOM	6496	CA	VAL	D	168	92.729	100.345	205.239	1.00	90.63	D
ATOM	6497	CB	VAL	D	168	93.031	99.628	206.578	1.00	90.94	D
ATOM	6498	CG1	VAL	D	168	94.050	98.524	206.354	1.00	92.62	D
ATOM	6499	CG2	VAL	D	168	93.551	100.620	207.603	1.00	89.65	D
ATOM	6500	C	VAL	D	168	93.907	101.250	204.867	1.00	84.92	D
ATOM	6501	O	VAL	D	168	95.061	100.961	205.186	1.00	84.46	D
ATOM	6502	N	THR	D	169	93.590	102.351	204.196	1.00	78.70	D
ATOM	6503	CA	THR	D	169	94.579	103.313	203.743	1.00	76.45	D
ATOM	6504	CB	THR	D	169	93.913	104.470	202.980	1.00	75.27	D
ATOM	6505	OG1	THR	D	169	93.420	103.984	201.728	1.00	77.62	D



ATOM	6506	CG2	THR	D	169	94.899	105.595	202.728	1.00	71.03	D
ATOM	6507	C	THR	D	169	95.413	103.913	204.852	1.00	76.86	D
ATOM	6508	O	THR	D	169	94.885	104.437	205.835	1.00	76.49	D
ATOM	6509	N	VAL	D	170	96.727	103.836	204.671	1.00	77.26	D
ATOM	6510	CA	VAL	D	170	97.668	104.391	205.629	1.00	78.22	D
ATOM	6511	CB	VAL	D	170	99.063	103.713	205.533	1.00	81.59	D
ATOM	6512	CG1	VAL	D	170	99.963	104.234	206.636	1.00	82.13	D
ATOM	6513	CG2	VAL	D	170	98.931	102.196	205.647	1.00	84.36	D
ATOM	6514	C	VAL	D	170	97.815	105.878	205.317	1.00	76.11	D
ATOM	6515	O	VAL	D	170	98.574	106.270	204.431	1.00	68.50	D
ATOM	6516	N	THR	D	171	97.049	106.692	206.038	1.00	79.42	D
ATOM	6517	CA	THR	D	171	97.074	108.138	205.883	1.00	81.52	D
ATOM	6518	CB	THR	D	171	95.830	108.799	206.575	1.00	77.65	D
ATOM	6519	OG1	THR	D	171	95.976	110.219	206.591	1.00	81.79	D
ATOM	6520	CG2	THR	D	171	95.686	108.336	207.997	1.00	73.42	D
ATOM	6521	C	THR	D	171	98.362	108.598	206.552	1.00	85.52	D
ATOM	6522	O	THR	D	171	98.392	109.612	207.251	1.00	88.94	D
ATOM	6523	N	LEU	D	172	99.433	107.845	206.318	1.00	86.85	D
ATOM	6524	CA	LEU	D	172	100.723	108.145	206.921	1.00	89.95	D
ATOM	6525	CB	LEU	D	172	101.691	106.962	206.721	1.00	94.36	D
ATOM	6526	CG	LEU	D	172	102.885	106.770	207.681	1.00	98.13	D
ATOM	6527	CD1	LEU	D	172	103.458	105.362	207.512	1.00	98.63	D
ATOM	6528	CD2	LEU	D	172	103.965	107.817	207.419	1.00	99.17	D
ATOM	6529	C	LEU	D	172	101.393	109.450	206.480	1.00	89.07	D
ATOM	6530	O	LEU	D	172	102.139	110.029	207.264	1.00	89.82	D
ATOM	6531	N	PRO	D	173	101.137	109.939	205.244	1.00	86.42	D
ATOM	6532	CD	PRO	D	173	100.015	109.681	204.328	1.00	84.78	D
ATOM	6533	CA	PRO	D	173	101.807	111.193	204.872	1.00	85.56	D
ATOM	6534	CB	PRO	D	173	100.976	111.694	203.688	1.00	81.87	D
ATOM	6535	CG	PRO	D	173	99.640	111.078	203.916	1.00	84.27	D
ATOM	6536	C	PRO	D	173	101.804	112.152	206.056	1.00	86.51	D
ATOM	6537	O	PRO	D	173	100.877	112.944	206.221	1.00	90.21	D
ATOM	6538	N	ASP	D	174	102.852	112.054	206.872	1.00	83.37	D
ATOM	6539	CA	ASP	D	174	103.002	112.837	208.091	1.00	81.03	D
ATOM	6540	CB	ASP	D	174	104.484	113.065	208.368	1.00	86.52	D
ATOM	6541	CG	ASP	D	174	105.222	111.761	208.609	1.00	89.39	D
ATOM	6542	OD1	ASP	D	174	105.414	110.999	207.635	1.00	90.18	D
ATOM	6543	OD2	ASP	D	174	105.591	111.487	209.775	1.00	96.23	D
ATOM	6544	C	ASP	D	174	102.213	114.131	208.134	1.00	76.73	D
ATOM	6545	O	ASP	D	174	102.131	114.861	207.148	1.00	72.49	D
ATOM	6546	N	TYR	D	175	101.638	114.389	209.304	1.00	73.53	D
ATOM	6547	CA	TYR	D	175	100.773	115.533	209.542	1.00	74.11	D
ATOM	6548	CB	TYR	D	175	101.288	116.427	210.666	1.00	72.91	D
ATOM	6549	CG	TYR	D	175	100.503	117.724	210.689	1.00	70.37	D
ATOM	6550	CD1	TYR	D	175	99.124	117.718	210.894	1.00	67.23	D
ATOM	6551	CE1	TYR	D	175	98.376	118.883	210.787	1.00	66.75	D
ATOM	6552	CD2	TYR	D	175	101.112	118.939	210.387	1.00	69.48	D
ATOM	6553	CE2	TYR	D	175	100.367	120.111	210.281	1.00	69.31	D
ATOM	6554	CZ	TYR	D	175	99.002	120.071	210.481	1.00	64.14	D
ATOM	6555	OH	TYR	D	175	98.268	121.220	210.371	1.00	65.72	D
ATOM	6556	C	TYR	D	175	100.381	116.445	208.384	1.00	74.39	D
ATOM	6557	O	TYR	D	175	99.196	116.676	208.161	1.00	81.52	D
ATOM	6558	N	PRO	D	176	101.347	117.015	207.655	1.00	66.94	D
ATOM	6559	CD	PRO	D	176	102.787	117.251	207.859	1.00	59.18	D
ATOM	6560	CA	PRO	D	176	100.810	117.868	206.588	1.00	61.40	D
ATOM	6561	CB	PRO	D	176	101.954	118.838	206.338	1.00	60.17	D
ATOM	6562	CG	PRO	D	176	103.162	117.956	206.587	1.00	64.68	D
ATOM	6563	C	PRO	D	176	100.362	117.135	205.315	1.00	55.87	D



ATOM	6564	O	PRO D 176	99.509	117.627	204.572	1.00	50.21	D
ATOM	6565	N	GLY D 177	100.935	115.956	205.092	1.00	54.90	D
ATOM	6566	CA	GLY D 177	100.649	115.165	203.902	1.00	55.03	D
ATOM	6567	C	GLY D 177	99.226	114.747	203.575	1.00	55.03	D
ATOM	6568	O	GLY D 177	98.361	114.693	204.448	1.00	59.29	D
ATOM	6569	N	SER D 178	98.998	114.431	202.301	1.00	49.88	D
ATOM	6570	CA	SER D 178	97.689	114.012	201.829	1.00	47.78	D
ATOM	6571	CB	SER D 178	96.922	115.213	201.269	1.00	43.67	D
ATOM	6572	OG	SER D 178	97.290	115.481	199.917	1.00	38.38	D
ATOM	6573	C	SER D 178	97.839	112.956	200.736	1.00	49.80	D
ATOM	6574	O	SER D 178	98.646	113.112	199.824	1.00	52.11	D
ATOM	6575	N	VAL D 179	97.065	111.878	200.820	1.00	51.59	D
ATOM	6576	CA	VAL D 179	97.153	110.833	199.806	1.00	52.35	D
ATOM	6577	CB	VAL D 179	97.391	109.419	200.402	1.00	48.88	D
ATOM	6578	CG1	VAL D 179	98.421	109.459	201.478	1.00	51.38	D
ATOM	6579	CG2	VAL D 179	96.092	108.860	200.934	1.00	53.47	D
ATOM	6580	C	VAL D 179	95.856	110.731	199.033	1.00	54.75	D
ATOM	6581	O	VAL D 179	94.819	111.273	199.447	1.00	54.64	D
ATOM	6582	N	PRO D 180	95.904	110.046	197.877	1.00	54.47	D
ATOM	6583	CD	PRO D 180	97.117	109.665	197.133	1.00	50.08	D
ATOM	6584	CA	PRO D 180	94.714	109.854	197.048	1.00	50.07	D
ATOM	6585	CB	PRO D 180	95.294	109.663	195.653	1.00	46.59	D
ATOM	6586	CG	PRO D 180	96.539	108.930	195.938	1.00	53.44	D
ATOM	6587	C	PRO D 180	94.094	108.586	197.623	1.00	44.18	D
ATOM	6588	O	PRO D 180	94.807	107.753	198.192	1.00	36.61	D
ATOM	6589	N	ILE D 181	92.776	108.466	197.516	1.00	45.45	D
ATOM	6590	CA	ILE D 181	92.067	107.307	198.045	1.00	43.31	D
ATOM	6591	CB	ILE D 181	90.937	107.709	198.974	1.00	44.06	D
ATOM	6592	CG2	ILE D 181	90.310	106.459	199.551	1.00	49.15	D
ATOM	6593	CG1	ILE D 181	91.468	108.596	200.097	1.00	44.53	D
ATOM	6594	CD1	ILE D 181	90.410	109.093	201.051	1.00	42.19	D
ATOM	6595	C	ILE D 181	91.465	106.480	196.935	1.00	44.63	D
ATOM	6596	O	ILE D 181	90.470	106.863	196.309	1.00	40.53	D
ATOM	6597	N	PRO D 182	92.062	105.317	196.679	1.00	47.10	D
ATOM	6598	CD	PRO D 182	93.200	104.733	197.402	1.00	47.00	D
ATOM	6599	CA	PRO D 182	91.585	104.417	195.633	1.00	45.23	D
ATOM	6600	CB	PRO D 182	92.615	103.296	195.639	1.00	48.60	D
ATOM	6601	CG	PRO D 182	93.826	103.914	196.333	1.00	50.26	D
ATOM	6602	C	PRO D 182	90.213	103.912	196.016	1.00	45.36	D
ATOM	6603	O	PRO D 182	90.049	103.247	197.040	1.00	43.34	D
ATOM	6604	N	LEU D 183	89.222	104.261	195.209	1.00	47.19	D
ATOM	6605	CA	LEU D 183	87.861	103.815	195.447	1.00	47.33	D
ATOM	6606	CB	LEU D 183	87.220	104.592	196.604	1.00	47.21	D
ATOM	6607	CG	LEU D 183	86.108	103.891	197.401	1.00	43.68	D
ATOM	6608	CD1	LEU D 183	85.680	104.759	198.568	1.00	43.88	D
ATOM	6609	CD2	LEU D 183	84.931	103.609	196.506	1.00	48.99	D
ATOM	6610	C	LEU D 183	87.080	104.034	194.163	1.00	48.03	D
ATOM	6611	O	LEU D 183	86.871	105.168	193.720	1.00	47.91	D
ATOM	6612	N	THR D 184	86.670	102.929	193.559	1.00	48.10	D
ATOM	6613	CA	THR D 184	85.908	102.969	192.324	1.00	46.87	D
ATOM	6614	CB	THR D 184	86.730	102.408	191.165	1.00	47.03	D
ATOM	6615	OG1	THR D 184	87.349	101.185	191.584	1.00	52.02	D
ATOM	6616	CG2	THR D 184	87.798	103.402	190.734	1.00	44.12	D
ATOM	6617	C	THR D 184	84.670	102.114	192.499	1.00	45.63	D
ATOM	6618	O	THR D 184	84.563	101.353	193.459	1.00	43.56	D
ATOM	6619	N	VAL D 185	83.731	102.258	191.579	1.00	44.30	D
ATOM	6620	CA	VAL D 185	82.515	101.478	191.624	1.00	49.34	D
ATOM	6621	CB	VAL D 185	81.328	102.252	192.258	1.00	50.55	D



ATOM	6622	CG1	VAL	D	185	81.619	102.549	193.690	1.00	60.81	D
ATOM	6623	CG2	VAL	D	185	81.065	103.546	191.506	1.00	49.78	D
ATOM	6624	C	VAL	D	185	82.108	101.118	190.215	1.00	50.78	D
ATOM	6625	O	VAL	D	185	82.223	101.937	189.295	1.00	47.23	D
ATOM	6626	N	TYR	D	186	81.650	99.886	190.040	1.00	51.36	D
ATOM	6627	CA	TYR	D	186	81.170	99.464	188.739	1.00	52.75	D
ATOM	6628	CB	TYR	D	186	82.181	98.558	188.028	1.00	48.03	D
ATOM	6629	CG	TYR	D	186	82.475	97.282	188.740	1.00	53.26	D
ATOM	6630	CD1	TYR	D	186	81.726	96.127	188.488	1.00	56.60	D
ATOM	6631	CE1	TYR	D	186	81.976	94.945	189.184	1.00	58.09	D
ATOM	6632	CD2	TYR	D	186	83.483	97.226	189.701	1.00	60.85	D
ATOM	6633	CE2	TYR	D	186	83.743	96.045	190.410	1.00	62.27	D
ATOM	6634	CZ	TYR	D	186	82.985	94.913	190.149	1.00	60.16	D
ATOM	6635	OH	TYR	D	186	83.214	93.769	190.879	1.00	61.60	D
ATOM	6636	C	TYR	D	186	79.863	98.752	188.994	1.00	51.88	D
ATOM	6637	O	TYR	D	186	79.628	98.252	190.094	1.00	48.23	D
ATOM	6638	N	CYS	D	187	79.002	98.755	187.984	1.00	54.13	D
ATOM	6639	CA	CYS	D	187	77.700	98.118	188.066	1.00	53.47	D
ATOM	6640	C	CYS	D	187	77.487	97.204	186.864	1.00	52.95	D
ATOM	6641	O	CYS	D	187	77.680	97.625	185.722	1.00	50.10	D
ATOM	6642	CB	CYS	D	187	76.588	99.167	188.052	1.00	52.28	D
ATOM	6643	SG	CYS	D	187	76.703	100.528	189.251	1.00	56.87	D
ATOM	6644	N	ALA	D	188	77.059	95.967	187.115	1.00	54.58	D
ATOM	6645	CA	ALA	D	188	76.790	95.023	186.028	1.00	50.96	D
ATOM	6646	CB	ALA	D	188	76.277	93.714	186.590	1.00	47.13	D
ATOM	6647	C	ALA	D	188	75.763	95.640	185.077	1.00	48.42	D
ATOM	6648	O	ALA	D	188	75.778	95.382	183.879	1.00	53.31	D
ATOM	6649	N	LYS	D	189	74.884	96.467	185.624	1.00	45.53	D
ATOM	6650	CA	LYS	D	189	73.870	97.155	184.841	1.00	48.59	D
ATOM	6651	CB	LYS	D	189	72.465	96.697	185.240	1.00	52.59	D
ATOM	6652	CG	LYS	D	189	72.240	95.190	185.223	1.00	55.87	D
ATOM	6653	CD	LYS	D	189	72.335	94.639	183.815	1.00	59.78	D
ATOM	6654	CE	LYS	D	189	71.318	95.288	182.880	1.00	57.69	D
ATOM	6655	NZ	LYS	D	189	71.566	94.886	181.463	1.00	57.35	D
ATOM	6656	C	LYS	D	189	74.006	98.639	185.162	1.00	52.27	D
ATOM	6657	O	LYS	D	189	73.936	99.034	186.328	1.00	57.31	D
ATOM	6658	N	SER	D	190	74.204	99.465	184.144	1.00	50.63	D
ATOM	6659	CA	SER	D	190	74.334	100.897	184.376	1.00	50.46	D
ATOM	6660	CB	SER	D	190	74.429	101.659	183.057	1.00	52.80	D
ATOM	6661	OG	SER	D	190	73.743	102.903	183.159	1.00	58.11	D
ATOM	6662	C	SER	D	190	73.161	101.449	185.174	1.00	47.62	D
ATOM	6663	O	SER	D	190	72.020	101.039	184.982	1.00	46.56	D
ATOM	6664	N	GLN	D	191	73.462	102.394	186.062	1.00	48.86	D
ATOM	6665	CA	GLN	D	191	72.452	103.035	186.904	1.00	44.46	D
ATOM	6666	CB	GLN	D	191	71.924	102.041	187.927	1.00	41.08	D
ATOM	6667	CG	GLN	D	191	73.006	101.393	188.755	1.00	47.69	D
ATOM	6668	CD	GLN	D	191	72.450	100.371	189.711	1.00	48.18	D
ATOM	6669	OE1	GLN	D	191	71.681	100.705	190.605	1.00	54.87	D
ATOM	6670	NE2	GLN	D	191	72.832	99.113	189.525	1.00	49.21	D
ATOM	6671	C	GLN	D	191	73.027	104.250	187.624	1.00	41.09	D
ATOM	6672	O	GLN	D	191	74.235	104.365	187.804	1.00	39.13	D
ATOM	6673	N	ASN	D	192	72.156	105.160	188.032	1.00	43.34	D
ATOM	6674	CA	ASN	D	192	72.604	106.353	188.733	1.00	44.26	D
ATOM	6675	CB	ASN	D	192	71.561	107.440	188.602	1.00	46.27	D
ATOM	6676	CG	ASN	D	192	71.172	107.673	187.173	1.00	56.10	D
ATOM	6677	OD1	ASN	D	192	72.033	107.720	186.281	1.00	58.79	D
ATOM	6678	ND2	ASN	D	192	69.871	107.824	186.931	1.00	62.26	D
ATOM	6679	C	ASN	D	192	72.901	106.111	190.203	1.00	44.03	D



ATOM	6680	O	ASN	D	192	72.087	105.564	190.947	1.00	50.24	D
ATOM	6681	N	LEU	D	193	74.084	106.527	190.618	1.00	40.97	D
ATOM	6682	CA	LEU	D	193	74.505	106.374	191.988	1.00	33.39	D
ATOM	6683	CB	LEU	D	193	75.758	105.505	192.080	1.00	29.92	D
ATOM	6684	CG	LEU	D	193	75.630	103.998	191.907	1.00	35.43	D
ATOM	6685	CD1	LEU	D	193	76.978	103.334	192.199	1.00	26.14	D
ATOM	6686	CD2	LEU	D	193	74.555	103.468	192.854	1.00	37.81	D
ATOM	6687	C	LEU	D	193	74.822	107.726	192.567	1.00	33.85	D
ATOM	6688	O	LEU	D	193	75.089	108.682	191.858	1.00	33.86	D
ATOM	6689	N	GLY	D	194	74.786	107.786	193.884	1.00	37.65	D
ATOM	6690	CA	GLY	D	194	75.107	108.996	194.597	1.00	36.81	D
ATOM	6691	C	GLY	D	194	75.708	108.504	195.891	1.00	35.13	D
ATOM	6692	O	GLY	D	194	75.471	107.353	196.275	1.00	33.04	D
ATOM	6693	N	TYR	D	195	76.509	109.328	196.555	1.00	32.62	D
ATOM	6694	CA	TYR	D	195	77.061	108.904	197.831	1.00	31.08	D
ATOM	6695	CB	TYR	D	195	78.407	108.218	197.647	1.00	30.68	D
ATOM	6696	CG	TYR	D	195	79.535	109.165	197.353	1.00	42.29	D
ATOM	6697	CD1	TYR	D	195	79.718	109.690	196.076	1.00	43.06	D
ATOM	6698	CE1	TYR	D	195	80.752	110.578	195.816	1.00	44.89	D
ATOM	6699	CD2	TYR	D	195	80.422	109.552	198.365	1.00	41.41	D
ATOM	6700	CE2	TYR	D	195	81.459	110.437	198.112	1.00	41.35	D
ATOM	6701	CZ	TYR	D	195	81.618	110.950	196.837	1.00	45.25	D
ATOM	6702	OH	TYR	D	195	82.625	111.855	196.584	1.00	46.12	D
ATOM	6703	C	TYR	D	195	77.207	110.056	198.805	1.00	29.69	D
ATOM	6704	O	TYR	D	195	77.140	111.229	198.430	1.00	30.55	D
ATOM	6705	N	TYR	D	196	77.355	109.709	200.074	1.00	29.95	D
ATOM	6706	CA	TYR	D	196	77.548	110.701	201.118	1.00	29.48	D
ATOM	6707	CB	TYR	D	196	76.217	111.262	201.645	1.00	28.82	D
ATOM	6708	CG	TYR	D	196	75.346	110.296	202.409	1.00	31.05	D
ATOM	6709	CD1	TYR	D	196	75.734	109.802	203.663	1.00	32.72	D
ATOM	6710	CE1	TYR	D	196	74.926	108.921	204.364	1.00	25.73	D
ATOM	6711	CD2	TYR	D	196	74.129	109.880	201.885	1.00	24.61	D
ATOM	6712	CE2	TYR	D	196	73.318	109.000	202.577	1.00	31.65	D
ATOM	6713	CZ	TYR	D	196	73.717	108.523	203.815	1.00	32.37	D
ATOM	6714	OH	TYR	D	196	72.885	107.662	204.485	1.00	29.82	D
ATOM	6715	C	TYR	D	196	78.334	110.054	202.235	1.00	26.69	D
ATOM	6716	O	TYR	D	196	78.292	108.829	202.419	1.00	22.17	D
ATOM	6717	N	LEU	D	197	79.086	110.895	202.939	1.00	26.36	D
ATOM	6718	CA	LEU	D	197	79.924	110.478	204.053	1.00	22.65	D
ATOM	6719	CB	LEU	D	197	81.182	111.329	204.092	1.00	21.09	D
ATOM	6720	CG	LEU	D	197	82.003	111.225	202.813	1.00	25.29	D
ATOM	6721	CD1	LEU	D	197	83.239	112.094	202.942	1.00	26.86	D
ATOM	6722	CD2	LEU	D	197	82.392	109.776	202.577	1.00	23.27	D
ATOM	6723	C	LEU	D	197	79.162	110.610	205.361	1.00	21.12	D
ATOM	6724	O	LEU	D	197	78.194	111.369	205.476	1.00	21.33	D
ATOM	6725	N	SER	D	198	79.619	109.874	206.356	1.00	18.32	D
ATOM	6726	CA	SER	D	198	78.964	109.873	207.649	1.00	18.41	D
ATOM	6727	CB	SER	D	198	77.862	108.828	207.639	1.00	19.24	D
ATOM	6728	OG	SER	D	198	78.447	107.536	207.501	1.00	26.22	D
ATOM	6729	C	SER	D	198	79.977	109.518	208.735	1.00	20.67	D
ATOM	6730	O	SER	D	198	80.834	108.649	208.545	1.00	14.54	D
ATOM	6731	N	GLY	D	199	79.856	110.182	209.879	1.00	22.31	D
ATOM	6732	CA	GLY	D	199	80.763	109.926	210.971	1.00	18.29	D
ATOM	6733	C	GLY	D	199	80.850	111.126	211.869	1.00	21.63	D
ATOM	6734	O	GLY	D	199	80.328	112.187	211.549	1.00	25.72	D
ATOM	6735	N	THR	D	200	81.517	110.953	213.001	1.00	27.65	D
ATOM	6736	CA	THR	D	200	81.685	112.019	213.986	1.00	28.35	D
ATOM	6737	CB	THR	D	200	82.337	111.476	215.246	1.00	26.26	D



ATOM	6738	OG1	THR	D	200	81.558	110.383	215.724	1.00	24.88	D
ATOM	6739	CG2	THR	D	200	82.408	112.541	216.309	1.00	26.91	D
ATOM	6740	C	THR	D	200	82.541	113.144	213.437	1.00	26.16	D
ATOM	6741	O	THR	D	200	83.631	112.920	212.948	1.00	25.10	D
ATOM	6742	N	THR	D	201	82.035	114.358	213.538	1.00	26.66	D
ATOM	6743	CA	THR	D	201	82.726	115.516	213.017	1.00	28.27	D
ATOM	6744	CB	THR	D	201	81.770	116.251	212.085	1.00	25.56	D
ATOM	6745	OG1	THR	D	201	82.054	115.858	210.739	1.00	25.73	D
ATOM	6746	CG2	THR	D	201	81.873	117.756	212.257	1.00	32.55	D
ATOM	6747	C	THR	D	201	83.274	116.453	214.100	1.00	29.04	D
ATOM	6748	O	THR	D	201	82.770	116.477	215.224	1.00	30.68	D
ATOM	6749	N	ALA	D	202	84.284	117.248	213.761	1.00	23.57	D
ATOM	6750	CA	ALA	D	202	84.867	118.122	214.762	1.00	25.46	D
ATOM	6751	CB	ALA	D	202	86.361	117.754	214.971	1.00	18.10	D
ATOM	6752	C	ALA	D	202	84.741	119.601	214.468	1.00	26.45	D
ATOM	6753	O	ALA	D	202	85.314	120.431	215.185	1.00	27.35	D
ATOM	6754	N	ASP	D	203	83.975	119.949	213.445	1.00	25.29	D
ATOM	6755	CA	ASP	D	203	83.859	121.355	213.067	1.00	22.97	D
ATOM	6756	CB	ASP	D	203	84.751	121.632	211.865	1.00	26.02	D
ATOM	6757	CG	ASP	D	203	84.453	120.709	210.692	1.00	31.30	D
ATOM	6758	OD1	ASP	D	203	84.272	121.204	209.563	1.00	35.99	D
ATOM	6759	OD2	ASP	D	203	84.395	119.478	210.892	1.00	35.08	D
ATOM	6760	C	ASP	D	203	82.459	121.776	212.720	1.00	23.55	D
ATOM	6761	O	ASP	D	203	81.618	120.940	212.423	1.00	24.97	D
ATOM	6762	N	ALA	D	204	82.217	123.081	212.747	1.00	23.32	D
ATOM	6763	CA	ALA	D	204	80.909	123.629	212.427	1.00	22.77	D
ATOM	6764	CB	ALA	D	204	80.897	125.099	212.701	1.00	12.66	D
ATOM	6765	C	ALA	D	204	80.538	123.365	210.964	1.00	28.34	D
ATOM	6766	O	ALA	D	204	79.354	123.272	210.620	1.00	34.32	D
ATOM	6767	N	GLY	D	205	81.545	123.246	210.107	1.00	27.24	D
ATOM	6768	CA	GLY	D	205	81.293	122.981	208.703	1.00	30.80	D
ATOM	6769	C	GLY	D	205	81.034	121.499	208.514	1.00	31.29	D
ATOM	6770	O	GLY	D	205	80.801	121.010	207.413	1.00	28.93	D
ATOM	6771	N	ASN	D	206	81.100	120.781	209.622	1.00	33.30	D
ATOM	6772	CA	ASN	D	206	80.833	119.359	209.634	1.00	34.62	D
ATOM	6773	CB	ASN	D	206	79.314	119.141	209.528	1.00	34.30	D
ATOM	6774	CG	ASN	D	206	78.914	117.693	209.726	1.00	41.52	D
ATOM	6775	OD1	ASN	D	206	78.180	117.127	208.916	1.00	46.41	D
ATOM	6776	ND2	ASN	D	206	79.390	117.084	210.806	1.00	37.73	D
ATOM	6777	C	ASN	D	206	81.577	118.566	208.558	1.00	31.76	D
ATOM	6778	O	ASN	D	206	81.035	117.626	207.997	1.00	33.42	D
ATOM	6779	N	SER	D	207	82.830	118.918	208.289	1.00	32.35	D
ATOM	6780	CA	SER	D	207	83.582	118.188	207.268	1.00	31.44	D
ATOM	6781	CB	SER	D	207	83.690	119.010	205.993	1.00	30.73	D
ATOM	6782	OG	SER	D	207	84.696	119.981	206.143	1.00	36.30	D
ATOM	6783	C	SER	D	207	84.978	117.728	207.663	1.00	30.24	D
ATOM	6784	O	SER	D	207	85.757	117.320	206.804	1.00	33.61	D
ATOM	6785	N	ILE	D	208	85.304	117.801	208.950	1.00	29.94	D
ATOM	6786	CA	ILE	D	208	86.611	117.342	209.449	1.00	28.43	D
ATOM	6787	CB	ILE	D	208	87.373	118.475	210.167	1.00	21.19	D
ATOM	6788	CG2	ILE	D	208	88.713	118.000	210.593	1.00	16.12	D
ATOM	6789	CG1	ILE	D	208	87.562	119.649	209.211	1.00	21.74	D
ATOM	6790	CD1	ILE	D	208	87.889	120.928	209.873	1.00	23.38	D
ATOM	6791	C	ILE	D	208	86.337	116.199	210.420	1.00	32.84	D
ATOM	6792	O	ILE	D	208	85.849	116.412	211.534	1.00	35.66	D
ATOM	6793	N	PHE	D	209	86.634	114.980	209.990	1.00	34.36	D
ATOM	6794	CA	PHE	D	209	86.353	113.826	210.819	1.00	36.28	D
ATOM	6795	CB	PHE	D	209	86.291	112.561	209.956	1.00	33.39	D



ATOM	6796	CG	PHE	D	209	85.113	112.542	209.018	1.00	30.28	D
ATOM	6797	CD1	PHE	D	209	85.184	113.171	207.779	1.00	30.91	D
ATOM	6798	CD2	PHE	D	209	83.890	112.004	209.429	1.00	34.03	D
ATOM	6799	CE1	PHE	D	209	84.054	113.276	206.960	1.00	32.18	D
ATOM	6800	CE2	PHE	D	209	82.751	112.101	208.624	1.00	35.54	D
ATOM	6801	CZ	PHE	D	209	82.833	112.743	207.384	1.00	35.20	D
ATOM	6802	C	PHE	D	209	87.268	113.639	212.002	1.00	41.75	D
ATOM	6803	O	PHE	D	209	88.481	113.514	211.869	1.00	49.71	D
ATOM	6804	N	THR	D	210	86.644	113.647	213.170	1.00	45.28	D
ATOM	6805	CA	THR	D	210	87.290	113.490	214.465	1.00	47.85	D
ATOM	6806	CB	THR	D	210	86.233	113.139	215.520	1.00	48.72	D
ATOM	6807	OG1	THR	D	210	85.458	114.307	215.808	1.00	53.11	D
ATOM	6808	CG2	THR	D	210	86.871	112.610	216.785	1.00	52.44	D
ATOM	6809	C	THR	D	210	88.387	112.438	214.516	1.00	50.24	D
ATOM	6810	O	THR	D	210	88.252	111.361	213.941	1.00	47.20	D
ATOM	6811	N	ASN	D	211	89.469	112.758	215.227	1.00	55.04	D
ATOM	6812	CA	ASN	D	211	90.573	111.824	215.368	1.00	56.56	D
ATOM	6813	CB	ASN	D	211	91.838	112.514	215.857	1.00	58.25	D
ATOM	6814	CG	ASN	D	211	93.002	111.537	216.022	1.00	60.84	D
ATOM	6815	OD1	ASN	D	211	94.102	111.926	216.414	1.00	66.22	D
ATOM	6816	ND2	ASN	D	211	92.762	110.264	215.718	1.00	54.74	D
ATOM	6817	C	ASN	D	211	90.211	110.744	216.356	1.00	56.12	D
ATOM	6818	O	ASN	D	211	90.004	111.006	217.530	1.00	54.01	D
ATOM	6819	N	THR	D	212	90.157	109.521	215.862	1.00	60.18	D
ATOM	6820	CA	THR	D	212	89.824	108.367	216.673	1.00	63.67	D
ATOM	6821	CB	THR	D	212	88.639	107.628	216.053	1.00	61.63	D
ATOM	6822	OG1	THR	D	212	87.441	108.359	216.329	1.00	58.04	D
ATOM	6823	CG2	THR	D	212	88.536	106.212	216.594	1.00	65.60	D
ATOM	6824	C	THR	D	212	91.021	107.430	216.757	1.00	68.00	D
ATOM	6825	O	THR	D	212	91.345	106.737	215.792	1.00	68.19	D
ATOM	6826	N	ALA	D	213	91.675	107.413	217.910	1.00	71.03	D
ATOM	6827	CA	ALA	D	213	92.838	106.566	218.111	1.00	73.96	D
ATOM	6828	CB	ALA	D	213	93.956	106.985	217.171	1.00	68.36	D
ATOM	6829	C	ALA	D	213	93.291	106.699	219.552	1.00	78.61	D
ATOM	6830	O	ALA	D	213	93.026	107.717	220.206	1.00	75.31	D
ATOM	6831	N	SER	D	214	93.974	105.670	220.046	1.00	85.62	D
ATOM	6832	CA	SER	D	214	94.461	105.686	221.418	1.00	92.04	D
ATOM	6833	CB	SER	D	214	94.284	104.309	222.057	1.00	91.32	D
ATOM	6834	OG	SER	D	214	94.434	104.390	223.465	1.00	96.07	D
ATOM	6835	C	SER	D	214	95.927	106.131	221.522	1.00	96.25	D
ATOM	6836	O	SER	D	214	96.210	107.173	222.124	1.00	94.70	D
ATOM	6837	N	PHE	D	215	96.847	105.364	220.931	1.00	100.55	D
ATOM	6838	CA	PHE	D	215	98.278	105.695	220.987	1.00	106.21	D
ATOM	6839	CB	PHE	D	215	99.060	104.976	219.877	1.00	114.06	D
ATOM	6840	CG	PHE	D	215	100.552	105.265	219.897	1.00	122.71	D
ATOM	6841	CD1	PHE	D	215	101.303	105.226	218.720	1.00	125.55	D
ATOM	6842	CD2	PHE	D	215	101.206	105.578	221.094	1.00	122.97	D
ATOM	6843	CE1	PHE	D	215	102.681	105.499	218.732	1.00	126.25	D
ATOM	6844	CE2	PHE	D	215	102.578	105.850	221.117	1.00	125.01	D
ATOM	6845	CZ	PHE	D	215	103.317	105.811	219.934	1.00	126.05	D
ATOM	6846	C	PHE	D	215	98.570	107.195	220.892	1.00	105.82	D
ATOM	6847	O	PHE	D	215	98.679	107.752	219.794	1.00	103.54	D
ATOM	6848	N	SER	D	216	98.728	107.825	222.053	1.00	106.12	D
ATOM	6849	CA	SER	D	216	99.002	109.253	222.141	1.00	105.35	D
ATOM	6850	CB	SER	D	216	100.508	109.519	222.110	1.00	107.35	D
ATOM	6851	OG	SER	D	216	100.776	110.887	222.375	1.00	109.15	D
ATOM	6852	C	SER	D	216	98.324	109.965	220.986	1.00	103.14	D
ATOM	6853	O	SER	D	216	98.916	110.174	219.925	1.00	104.74	D



ATOM	6854	N	PRO	D	217	97.060	110.349	221.183	1.00	99.73	D
ATOM	6855	CD	PRO	D	217	96.344	110.325	222.469	1.00	99.02	D
ATOM	6856	CA	PRO	D	217	96.269	111.041	220.166	1.00	96.62	D
ATOM	6857	CB	PRO	D	217	94.924	111.237	220.859	1.00	98.45	D
ATOM	6858	CG	PRO	D	217	95.329	111.431	222.284	1.00	98.16	D
ATOM	6859	C	PRO	D	217	96.857	112.361	219.694	1.00	90.70	D
ATOM	6860	O	PRO	D	217	96.718	113.378	220.369	1.00	89.52	D
ATOM	6861	N	ALA	D	218	97.521	112.339	218.543	1.00	83.37	D
ATOM	6862	CA	ALA	D	218	98.072	113.561	217.996	1.00	79.95	D
ATOM	6863	CB	ALA	D	218	98.577	113.324	216.589	1.00	77.78	D
ATOM	6864	C	ALA	D	218	96.895	114.531	217.977	1.00	78.09	D
ATOM	6865	O	ALA	D	218	96.160	114.611	216.994	1.00	83.21	D
ATOM	6866	N	GLN	D	219	96.714	115.259	219.070	1.00	72.86	D
ATOM	6867	CA	GLN	D	219	95.605	116.194	219.193	1.00	71.16	D
ATOM	6868	CB	GLN	D	219	95.525	116.715	220.622	1.00	73.68	D
ATOM	6869	CG	GLN	D	219	94.405	117.709	220.821	1.00	81.65	D
ATOM	6870	CD	GLN	D	219	94.471	118.381	222.163	1.00	87.94	D
ATOM	6871	OE1	GLN	D	219	93.629	119.222	222.497	1.00	91.13	D
ATOM	6872	NE2	GLN	D	219	95.477	118.015	222.954	1.00	92.41	D
ATOM	6873	C	GLN	D	219	95.645	117.390	218.254	1.00	67.43	D
ATOM	6874	O	GLN	D	219	96.708	117.791	217.793	1.00	65.06	D
ATOM	6875	N	GLY	D	220	94.467	117.950	217.978	1.00	66.01	D
ATOM	6876	CA	GLY	D	220	94.368	119.133	217.134	1.00	63.87	D
ATOM	6877	C	GLY	D	220	94.193	118.993	215.632	1.00	61.04	D
ATOM	6878	O	GLY	D	220	93.949	119.994	214.948	1.00	58.72	D
ATOM	6879	N	VAL	D	221	94.303	117.774	215.108	1.00	57.83	D
ATOM	6880	CA	VAL	D	221	94.166	117.585	213.677	1.00	54.92	D
ATOM	6881	CB	VAL	D	221	95.301	116.701	213.123	1.00	53.92	D
ATOM	6882	CG1	VAL	D	221	95.418	116.889	211.615	1.00	53.17	D
ATOM	6883	CG2	VAL	D	221	96.598	117.059	213.785	1.00	50.61	D
ATOM	6884	C	VAL	D	221	92.811	117.014	213.250	1.00	54.08	D
ATOM	6885	O	VAL	D	221	91.775	117.595	213.551	1.00	55.95	D
ATOM	6886	N	GLY	D	222	92.821	115.885	212.546	1.00	50.29	D
ATOM	6887	CA	GLY	D	222	91.584	115.295	212.061	1.00	45.40	D
ATOM	6888	C	GLY	D	222	91.646	115.107	210.553	1.00	39.80	D
ATOM	6889	O	GLY	D	222	92.304	115.872	209.863	1.00	41.10	D
ATOM	6890	N	VAL	D	223	90.958	114.092	210.049	1.00	34.73	D
ATOM	6891	CA	VAL	D	223	90.935	113.759	208.622	1.00	32.14	D
ATOM	6892	CB	VAL	D	223	90.848	112.234	208.442	1.00	35.22	D
ATOM	6893	CG1	VAL	D	223	90.681	111.888	206.981	1.00	34.40	D
ATOM	6894	CG2	VAL	D	223	92.084	111.577	209.024	1.00	32.82	D
ATOM	6895	C	VAL	D	223	89.786	114.384	207.826	1.00	30.52	D
ATOM	6896	O	VAL	D	223	88.630	114.339	208.252	1.00	30.39	D
ATOM	6897	N	GLN	D	224	90.106	114.955	206.665	1.00	29.44	D
ATOM	6898	CA	GLN	D	224	89.091	115.577	205.810	1.00	31.99	D
ATOM	6899	CB	GLN	D	224	89.274	117.087	205.759	1.00	22.25	D
ATOM	6900	CG	GLN	D	224	88.141	117.819	205.084	1.00	29.08	D
ATOM	6901	CD	GLN	D	224	88.441	119.302	204.895	1.00	36.59	D
ATOM	6902	OE1	GLN	D	224	87.562	120.150	205.022	1.00	42.00	D
ATOM	6903	NE2	GLN	D	224	89.687	119.617	204.580	1.00	39.93	D
ATOM	6904	C	GLN	D	224	89.226	114.996	204.410	1.00	35.66	D
ATOM	6905	O	GLN	D	224	90.336	114.856	203.900	1.00	37.26	D
ATOM	6906	N	LEU	D	225	88.103	114.641	203.792	1.00	35.79	D
ATOM	6907	CA	LEU	D	225	88.150	114.050	202.465	1.00	30.99	D
ATOM	6908	CB	LEU	D	225	87.223	112.838	202.377	1.00	27.28	D
ATOM	6909	CG	LEU	D	225	87.515	111.727	203.386	1.00	33.61	D
ATOM	6910	CD1	LEU	D	225	86.789	110.453	202.992	1.00	33.10	D
ATOM	6911	CD2	LEU	D	225	89.004	111.466	203.446	1.00	36.51	D



ATOM	6912	C	LEU	D	225	87.804	115.054	201.394	1.00	31.00	D
ATOM	6913	O	LEU	D	225	86.932	115.917	201.551	1.00	32.09	D
ATOM	6914	N	THR	D	226	88.489	114.912	200.276	1.00	28.47	D
ATOM	6915	CA	THR	D	226	88.296	115.828	199.187	1.00	25.76	D
ATOM	6916	CB	THR	D	226	89.508	116.780	199.202	1.00	23.32	D
ATOM	6917	OG1	THR	D	226	89.146	118.041	198.642	1.00	29.32	D
ATOM	6918	CG2	THR	D	226	90.675	116.154	198.478	1.00	18.21	D
ATOM	6919	C	THR	D	226	88.145	115.037	197.866	1.00	25.30	D
ATOM	6920	O	THR	D	226	88.670	113.919	197.729	1.00	20.99	D
ATOM	6921	N	ARG	D	227	87.381	115.591	196.925	1.00	26.38	D
ATOM	6922	CA	ARG	D	227	87.172	114.946	195.618	1.00	31.47	D
ATOM	6923	CB	ARG	D	227	85.683	114.524	195.425	1.00	23.83	D
ATOM	6924	CG	ARG	D	227	84.663	115.657	195.516	1.00	22.21	D
ATOM	6925	CD	ARG	D	227	83.213	115.165	195.393	1.00	30.01	D
ATOM	6926	NE	ARG	D	227	82.335	116.163	194.765	1.00	26.28	D
ATOM	6927	CZ	ARG	D	227	81.529	116.984	195.417	1.00	30.20	D
ATOM	6928	NH1	ARG	D	227	81.463	116.934	196.744	1.00	37.40	D
ATOM	6929	NH2	ARG	D	227	80.817	117.877	194.741	1.00	29.17	D
ATOM	6930	C	ARG	D	227	87.629	115.951	194.549	1.00	33.56	D
ATOM	6931	O	ARG	D	227	86.909	116.904	194.204	1.00	26.33	D
ATOM	6932	N	ASN	D	228	88.847	115.728	194.047	1.00	39.95	D
ATOM	6933	CA	ASN	D	228	89.469	116.628	193.068	1.00	42.75	D
ATOM	6934	CB	ASN	D	228	88.761	116.534	191.716	1.00	47.73	D
ATOM	6935	CG	ASN	D	228	89.106	115.265	190.975	1.00	56.00	D
ATOM	6936	OD1	ASN	D	228	88.896	115.171	189.771	1.00	68.18	D
ATOM	6937	ND2	ASN	D	228	89.641	114.276	191.690	1.00	55.97	D
ATOM	6938	C	ASN	D	228	89.434	118.068	193.578	1.00	40.30	D
ATOM	6939	O	ASN	D	228	88.976	118.982	192.894	1.00	39.54	D
ATOM	6940	N	GLY	D	229	89.884	118.257	194.809	1.00	39.42	D
ATOM	6941	CA	GLY	D	229	89.901	119.587	195.379	1.00	42.64	D
ATOM	6942	C	GLY	D	229	88.668	120.042	196.141	1.00	44.99	D
ATOM	6943	O	GLY	D	229	88.770	120.935	196.992	1.00	46.97	D
ATOM	6944	N	THR	D	230	87.507	119.463	195.841	1.00	42.99	D
ATOM	6945	CA	THR	D	230	86.281	119.855	196.526	1.00	41.26	D
ATOM	6946	CB	THR	D	230	85.046	119.573	195.683	1.00	42.11	D
ATOM	6947	OG1	THR	D	230	85.012	120.479	194.581	1.00	43.56	D
ATOM	6948	CG2	THR	D	230	83.781	119.755	196.512	1.00	42.63	D
ATOM	6949	C	THR	D	230	86.134	119.094	197.826	1.00	43.32	D
ATOM	6950	O	THR	D	230	86.321	117.872	197.868	1.00	47.88	D
ATOM	6951	N	ILE	D	231	85.796	119.822	198.883	1.00	36.94	D
ATOM	6952	CA	ILE	D	231	85.629	119.228	200.195	1.00	33.80	D
ATOM	6953	CB	ILE	D	231	85.663	120.312	201.304	1.00	38.72	D
ATOM	6954	CG2	ILE	D	231	85.190	119.730	202.643	1.00	33.72	D
ATOM	6955	CG1	ILE	D	231	87.075	120.877	201.442	1.00	33.42	D
ATOM	6956	CD1	ILE	D	231	87.176	121.972	202.484	1.00	39.63	D
ATOM	6957	C	ILE	D	231	84.304	118.503	200.272	1.00	30.75	D
ATOM	6958	O	ILE	D	231	83.294	118.964	199.746	1.00	30.78	D
ATOM	6959	N	ILE	D	232	84.311	117.363	200.940	1.00	28.89	D
ATOM	6960	CA	ILE	D	232	83.091	116.596	201.088	1.00	28.70	D
ATOM	6961	CB	ILE	D	232	83.302	115.145	200.609	1.00	28.24	D
ATOM	6962	CG2	ILE	D	232	81.991	114.361	200.693	1.00	22.26	D
ATOM	6963	CG1	ILE	D	232	83.829	115.146	199.168	1.00	27.91	D
ATOM	6964	CD1	ILE	D	232	84.373	113.809	198.717	1.00	13.19	D
ATOM	6965	C	ILE	D	232	82.620	116.577	202.544	1.00	29.44	D
ATOM	6966	O	ILE	D	232	83.144	115.828	203.368	1.00	33.08	D
ATOM	6967	N	PRO	D	233	81.665	117.448	202.895	1.00	25.35	D
ATOM	6968	CD	PRO	D	233	81.277	118.701	202.234	1.00	18.19	D
ATOM	6969	CA	PRO	D	233	81.199	117.418	204.285	1.00	27.11	D



ATOM	6970	CB	PRO	D	233	80.463	118.755	204.438	1.00	28.32	D
ATOM	6971	CG	PRO	D	233	80.099	119.131	203.041	1.00	23.27	D
ATOM	6972	C	PRO	D	233	80.274	116.212	204.482	1.00	28.07	D
ATOM	6973	O	PRO	D	233	79.661	115.730	203.527	1.00	29.41	D
ATOM	6974	N	ALA	D	234	80.191	115.721	205.711	1.00	25.19	D
ATOM	6975	CA	ALA	D	234	79.336	114.577	206.032	1.00	24.45	D
ATOM	6976	CB	ALA	D	234	79.416	114.284	207.500	1.00	23.54	D
ATOM	6977	C	ALA	D	234	77.886	114.833	205.651	1.00	23.36	D
ATOM	6978	O	ALA	D	234	77.388	115.947	205.826	1.00	22.76	D
ATOM	6979	N	ASN	D	235	77.217	113.810	205.115	1.00	20.29	D
ATOM	6980	CA	ASN	D	235	75.806	113.928	204.735	1.00	24.03	D
ATOM	6981	CB	ASN	D	235	74.971	114.198	205.987	1.00	21.15	D
ATOM	6982	CG	ASN	D	235	75.234	113.170	207.065	1.00	31.43	D
ATOM	6983	OD1	ASN	D	235	75.760	113.482	208.137	1.00	30.92	D
ATOM	6984	ND2	ASN	D	235	74.899	111.921	206.772	1.00	27.98	D
ATOM	6985	C	ASN	D	235	75.487	114.970	203.662	1.00	27.38	D
ATOM	6986	O	ASN	D	235	74.495	115.689	203.749	1.00	29.05	D
ATOM	6987	N	ASN	D	236	76.348	115.040	202.656	1.00	28.27	D
ATOM	6988	CA	ASN	D	236	76.198	115.943	201.524	1.00	28.78	D
ATOM	6989	CB	ASN	D	236	77.374	116.927	201.467	1.00	40.66	D
ATOM	6990	CG	ASN	D	236	77.433	117.714	200.156	1.00	42.40	D
ATOM	6991	OD1	ASN	D	236	76.497	118.424	199.804	1.00	44.46	D
ATOM	6992	ND2	ASN	D	236	78.544	117.585	199.433	1.00	48.38	D
ATOM	6993	C	ASN	D	236	76.261	114.981	200.351	1.00	30.86	D
ATOM	6994	O	ASN	D	236	77.338	114.524	199.987	1.00	35.00	D
ATOM	6995	N	THR	D	237	75.121	114.659	199.757	1.00	27.03	D
ATOM	6996	CA	THR	D	237	75.131	113.692	198.677	1.00	29.29	D
ATOM	6997	CB	THR	D	237	73.689	113.232	198.317	1.00	32.75	D
ATOM	6998	OG1	THR	D	237	72.958	112.933	199.517	1.00	38.08	D
ATOM	6999	CG2	THR	D	237	73.743	111.973	197.476	1.00	31.75	D
ATOM	7000	C	THR	D	237	75.848	114.143	197.418	1.00	30.23	D
ATOM	7001	O	THR	D	237	75.527	115.179	196.832	1.00	30.08	D
ATOM	7002	N	VAL	D	238	76.839	113.353	197.019	1.00	30.79	D
ATOM	7003	CA	VAL	D	238	77.601	113.632	195.812	1.00	34.92	D
ATOM	7004	CB	VAL	D	238	79.102	113.331	195.985	1.00	38.68	D
ATOM	7005	CG1	VAL	D	238	79.805	113.353	194.623	1.00	37.66	D
ATOM	7006	CG2	VAL	D	238	79.730	114.356	196.897	1.00	48.14	D
ATOM	7007	C	VAL	D	238	77.068	112.726	194.720	1.00	36.74	D
ATOM	7008	O	VAL	D	238	77.114	111.494	194.835	1.00	35.04	D
ATOM	7009	N	SER	D	239	76.574	113.340	193.658	1.00	38.11	D
ATOM	7010	CA	SER	D	239	76.028	112.586	192.551	1.00	40.31	D
ATOM	7011	CB	SER	D	239	75.026	113.427	191.790	1.00	43.12	D
ATOM	7012	OG	SER	D	239	74.560	112.686	190.685	1.00	57.96	D
ATOM	7013	C	SER	D	239	77.070	112.095	191.575	1.00	38.99	D
ATOM	7014	O	SER	D	239	77.750	112.888	190.936	1.00	43.11	D
ATOM	7015	N	LEU	D	240	77.170	110.781	191.446	1.00	37.87	D
ATOM	7016	CA	LEU	D	240	78.118	110.149	190.531	1.00	37.49	D
ATOM	7017	CB	LEU	D	240	78.456	108.754	191.040	1.00	30.98	D
ATOM	7018	CG	LEU	D	240	79.460	108.698	192.179	1.00	31.09	D
ATOM	7019	CD1	LEU	D	240	79.540	107.275	192.688	1.00	35.18	D
ATOM	7020	CD2	LEU	D	240	80.814	109.170	191.697	1.00	20.40	D
ATOM	7021	C	LEU	D	240	77.630	110.034	189.078	1.00	38.52	D
ATOM	7022	O	LEU	D	240	78.412	109.725	188.180	1.00	33.90	D
ATOM	7023	N	GLY	D	241	76.341	110.279	188.857	1.00	42.42	D
ATOM	7024	CA	GLY	D	241	75.778	110.164	187.522	1.00	44.14	D
ATOM	7025	C	GLY	D	241	75.512	108.701	187.190	1.00	45.64	D
ATOM	7026	O	GLY	D	241	75.135	107.924	188.067	1.00	43.50	D
ATOM	7027	N	ALA	D	242	75.711	108.318	185.931	1.00	46.01	D



ATOM	7028	CA	ALA	D	242	75.504	106.934	185.534	1.00	44.50	D
ATOM	7029	CB	ALA	D	242	75.015	106.861	184.119	1.00	44.60	D
ATOM	7030	C	ALA	D	242	76.802	106.168	185.669	1.00	44.15	D
ATOM	7031	O	ALA	D	242	77.841	106.599	185.174	1.00	44.58	D
ATOM	7032	N	VAL	D	243	76.738	105.039	186.360	1.00	44.23	D
ATOM	7033	CA	VAL	D	243	77.903	104.199	186.556	1.00	46.51	D
ATOM	7034	CB	VAL	D	243	78.184	103.981	188.038	1.00	43.76	D
ATOM	7035	CG1	VAL	D	243	79.424	103.115	188.212	1.00	43.46	D
ATOM	7036	CG2	VAL	D	243	78.362	105.313	188.710	1.00	50.13	D
ATOM	7037	C	VAL	D	243	77.590	102.861	185.903	1.00	49.53	D
ATOM	7038	O	VAL	D	243	76.536	102.272	186.158	1.00	53.02	D
ATOM	7039	N	GLY	D	244	78.505	102.391	185.062	1.00	45.58	D
ATOM	7040	CA	GLY	D	244	78.290	101.140	184.379	1.00	43.81	D
ATOM	7041	C	GLY	D	244	79.364	100.095	184.580	1.00	47.30	D
ATOM	7042	O	GLY	D	244	79.917	99.938	185.676	1.00	47.49	D
ATOM	7043	N	THR	D	245	79.666	99.381	183.500	1.00	50.57	D
ATOM	7044	CA	THR	D	245	80.642	98.299	183.534	1.00	51.81	D
ATOM	7045	CB	THR	D	245	80.520	97.424	182.260	1.00	51.13	D
ATOM	7046	OG1	THR	D	245	80.552	98.253	181.090	1.00	55.23	D
ATOM	7047	CG2	THR	D	245	79.200	96.661	182.284	1.00	46.04	D
ATOM	7048	C	THR	D	245	82.073	98.756	183.742	1.00	50.91	D
ATOM	7049	O	THR	D	245	82.905	98.003	184.253	1.00	53.14	D
ATOM	7050	N	SER	D	246	82.359	99.993	183.352	1.00	51.11	D
ATOM	7051	CA	SER	D	246	83.695	100.550	183.538	1.00	50.38	D
ATOM	7052	CB	SER	D	246	84.020	101.577	182.452	1.00	49.82	D
ATOM	7053	OG	SER	D	246	83.704	101.083	181.165	1.00	57.34	D
ATOM	7054	C	SER	D	246	83.681	101.244	184.895	1.00	47.94	D
ATOM	7055	O	SER	D	246	82.831	102.103	185.151	1.00	47.72	D
ATOM	7056	N	ALA	D	247	84.611	100.861	185.760	1.00	44.78	D
ATOM	7057	CA	ALA	D	247	84.713	101.449	187.086	1.00	45.33	D
ATOM	7058	CB	ALA	D	247	85.910	100.866	187.815	1.00	44.79	D
ATOM	7059	C	ALA	D	247	84.827	102.974	187.041	1.00	46.03	D
ATOM	7060	O	ALA	D	247	85.380	103.550	186.108	1.00	48.87	D
ATOM	7061	N	VAL	D	248	84.287	103.621	188.058	1.00	44.62	D
ATOM	7062	CA	VAL	D	248	84.336	105.062	188.156	1.00	45.32	D
ATOM	7063	CB	VAL	D	248	82.929	105.677	188.183	1.00	46.30	D
ATOM	7064	CG1	VAL	D	248	83.013	107.153	188.532	1.00	42.83	D
ATOM	7065	CG2	VAL	D	248	82.259	105.485	186.845	1.00	44.21	D
ATOM	7066	C	VAL	D	248	85.028	105.394	189.460	1.00	48.91	D
ATOM	7067	O	VAL	D	248	84.614	104.931	190.527	1.00	51.75	D
ATOM	7068	N	SER	D	249	86.086	106.191	189.366	1.00	48.11	D
ATOM	7069	CA	SER	D	249	86.851	106.602	190.532	1.00	45.35	D
ATOM	7070	CB	SER	D	249	88.257	107.022	190.103	1.00	42.10	D
ATOM	7071	OG	SER	D	249	89.078	107.301	191.219	1.00	39.95	D
ATOM	7072	C	SER	D	249	86.139	107.780	191.177	1.00	44.60	D
ATOM	7073	O	SER	D	249	85.744	108.708	190.482	1.00	42.89	D
ATOM	7074	N	LEU	D	250	85.956	107.744	192.494	1.00	45.11	D
ATOM	7075	CA	LEU	D	250	85.303	108.868	193.172	1.00	46.11	D
ATOM	7076	CB	LEU	D	250	84.861	108.490	194.592	1.00	48.42	D
ATOM	7077	CG	LEU	D	250	83.945	107.277	194.789	1.00	51.17	D
ATOM	7078	CD1	LEU	D	250	83.407	107.308	196.226	1.00	46.15	D
ATOM	7079	CD2	LEU	D	250	82.798	107.303	193.768	1.00	45.53	D
ATOM	7080	C	LEU	D	250	86.289	110.032	193.243	1.00	45.02	D
ATOM	7081	O	LEU	D	250	85.904	111.171	193.517	1.00	41.99	D
ATOM	7082	N	GLY	D	251	87.562	109.726	192.991	1.00	39.63	D
ATOM	7083	CA	GLY	D	251	88.592	110.741	193.022	1.00	39.22	D
ATOM	7084	C	GLY	D	251	88.745	111.335	194.402	1.00	39.04	D
ATOM	7085	O	GLY	D	251	88.757	112.560	194.574	1.00	43.58	D



ATOM	7086	N	LEU	D	252	88.871	110.458	195.385	1.00	34.35	D
ATOM	7087	CA	LEU	D	252	88.999	110.878	196.765	1.00	36.45	D
ATOM	7088	CB	LEU	D	252	88.311	109.867	197.688	1.00	35.74	D
ATOM	7089	CG	LEU	D	252	86.802	109.663	197.565	1.00	31.39	D
ATOM	7090	CD1	LEU	D	252	86.409	108.508	198.451	1.00	28.23	D
ATOM	7091	CD2	LEU	D	252	86.066	110.922	197.949	1.00	27.38	D
ATOM	7092	C	LEU	D	252	90.431	111.034	197.227	1.00	35.68	D
ATOM	7093	O	LEU	D	252	91.325	110.342	196.764	1.00	40.05	D
ATOM	7094	N	THR	D	253	90.639	111.959	198.150	1.00	34.52	D
ATOM	7095	CA	THR	D	253	91.952	112.175	198.743	1.00	35.10	D
ATOM	7096	CB	THR	D	253	92.680	113.384	198.142	1.00	37.63	D
ATOM	7097	OG1	THR	D	253	93.359	112.979	196.950	1.00	42.09	D
ATOM	7098	CG2	THR	D	253	93.686	113.950	199.128	1.00	24.76	D
ATOM	7099	C	THR	D	253	91.732	112.460	200.210	1.00	35.90	D
ATOM	7100	O	THR	D	253	90.820	113.226	200.569	1.00	34.87	D
ATOM	7101	N	ALA	D	254	92.543	111.829	201.056	1.00	31.41	D
ATOM	7102	CA	ALA	D	254	92.454	112.069	202.490	1.00	32.89	D
ATOM	7103	CB	ALA	D	254	92.915	110.841	203.274	1.00	22.29	D
ATOM	7104	C	ALA	D	254	93.367	113.272	202.787	1.00	38.15	D
ATOM	7105	O	ALA	D	254	94.504	113.350	202.306	1.00	40.40	D
ATOM	7106	N	ASN	D	255	92.857	114.210	203.572	1.00	39.54	D
ATOM	7107	CA	ASN	D	255	93.601	115.409	203.938	1.00	38.37	D
ATOM	7108	CB	ASN	D	255	92.968	116.634	203.301	1.00	32.80	D
ATOM	7109	CG	ASN	D	255	92.876	116.529	201.827	1.00	31.80	D
ATOM	7110	OD1	ASN	D	255	93.721	117.044	201.113	1.00	36.08	D
ATOM	7111	ND2	ASN	D	255	91.843	115.862	201.346	1.00	39.71	D
ATOM	7112	C	ASN	D	255	93.542	115.627	205.430	1.00	38.87	D
ATOM	7113	O	ASN	D	255	92.548	115.278	206.066	1.00	42.12	D
ATOM	7114	N	TYR	D	256	94.595	116.207	205.994	1.00	39.04	D
ATOM	7115	CA	TYR	D	256	94.564	116.539	207.414	1.00	36.05	D
ATOM	7116	CB	TYR	D	256	95.955	116.540	208.036	1.00	32.41	D
ATOM	7117	CG	TYR	D	256	96.643	115.202	208.152	1.00	29.12	D
ATOM	7118	CD1	TYR	D	256	97.672	114.847	207.270	1.00	28.62	D
ATOM	7119	CE1	TYR	D	256	98.392	113.668	207.429	1.00	31.66	D
ATOM	7120	CD2	TYR	D	256	96.338	114.332	209.192	1.00	28.02	D
ATOM	7121	CE2	TYR	D	256	97.044	113.143	209.365	1.00	32.95	D
ATOM	7122	CZ	TYR	D	256	98.075	112.813	208.483	1.00	37.34	D
ATOM	7123	OH	TYR	D	256	98.787	111.643	208.653	1.00	30.52	D
ATOM	7124	C	TYR	D	256	94.012	117.969	207.471	1.00	35.46	D
ATOM	7125	O	TYR	D	256	94.352	118.813	206.639	1.00	37.11	D
ATOM	7126	N	ALA	D	257	93.133	118.231	208.423	1.00	35.88	D
ATOM	7127	CA	ALA	D	257	92.576	119.564	208.597	1.00	36.41	D
ATOM	7128	CB	ALA	D	257	91.119	119.585	208.217	1.00	35.53	D
ATOM	7129	C	ALA	D	257	92.740	119.856	210.077	1.00	41.40	D
ATOM	7130	O	ALA	D	257	92.869	118.940	210.894	1.00	41.85	D
ATOM	7131	N	ARG	D	258	92.762	121.125	210.438	1.00	47.81	D
ATOM	7132	CA	ARG	D	258	92.924	121.461	211.844	1.00	53.13	D
ATOM	7133	CB	ARG	D	258	93.823	122.688	212.007	1.00	57.05	D
ATOM	7134	CG	ARG	D	258	95.267	122.482	211.604	1.00	59.44	D
ATOM	7135	CD	ARG	D	258	96.005	123.794	211.712	1.00	70.48	D
ATOM	7136	NE	ARG	D	258	95.959	124.318	213.075	1.00	79.47	D
ATOM	7137	CZ	ARG	D	258	96.187	125.588	213.393	1.00	83.17	D
ATOM	7138	NH1	ARG	D	258	96.471	126.469	212.442	1.00	86.75	D
ATOM	7139	NH2	ARG	D	258	96.137	125.978	214.660	1.00	86.31	D
ATOM	7140	C	ARG	D	258	91.574	121.733	212.479	1.00	53.99	D
ATOM	7141	O	ARG	D	258	90.742	122.467	211.922	1.00	53.11	D
ATOM	7142	N	THR	D	259	91.377	121.140	213.652	1.00	54.62	D
ATOM	7143	CA	THR	D	259	90.145	121.283	214.409	1.00	57.01	D



ATOM	7144	CB	THR	D	259	89.868	120.037	215.231	1.00	56.62	D
ATOM	7145	OG1	THR	D	259	91.048	119.673	215.956	1.00	63.13	D
ATOM	7146	CG2	THR	D	259	89.469	118.896	214.336	1.00	62.99	D
ATOM	7147	C	THR	D	259	90.234	122.445	215.366	1.00	60.43	D
ATOM	7148	O	THR	D	259	89.789	123.551	215.058	1.00	58.62	D
ATOM	7149	N	GLY	D	260	90.823	122.169	216.529	1.00	66.46	D
ATOM	7150	CA	GLY	D	260	90.988	123.167	217.571	1.00	69.32	D
ATOM	7151	C	GLY	D	260	92.031	124.215	217.254	1.00	70.64	D
ATOM	7152	O	GLY	D	260	91.863	125.003	216.324	1.00	70.48	D
ATOM	7153	N	GLY	D	261	93.112	124.229	218.026	1.00	73.69	D
ATOM	7154	CA	GLY	D	261	94.163	125.210	217.791	1.00	75.92	D
ATOM	7155	C	GLY	D	261	95.563	124.616	217.747	1.00	77.22	D
ATOM	7156	O	GLY	D	261	96.115	124.375	216.671	1.00	78.84	D
ATOM	7157	N	GLN	D	262	96.141	124.374	218.916	1.00	76.59	D
ATOM	7158	CA	GLN	D	262	97.479	123.813	218.997	1.00	77.05	D
ATOM	7159	CB	GLN	D	262	97.961	123.849	220.448	1.00	85.73	D
ATOM	7160	CG	GLN	D	262	99.474	123.779	220.649	1.00	93.06	D
ATOM	7161	CD	GLN	D	262	100.160	125.096	220.326	1.00	97.67	D
ATOM	7162	OE1	GLN	D	262	101.184	125.439	220.926	1.00	99.48	D
ATOM	7163	NE2	GLN	D	262	99.602	125.840	219.367	1.00	99.46	D
ATOM	7164	C	GLN	D	262	97.503	122.372	218.501	1.00	72.22	D
ATOM	7165	O	GLN	D	262	96.826	121.504	219.057	1.00	72.19	D
ATOM	7166	N	VAL	D	263	98.279	122.122	217.454	1.00	65.55	D
ATOM	7167	CA	VAL	D	263	98.397	120.776	216.926	1.00	60.92	D
ATOM	7168	CB	VAL	D	263	98.876	120.796	215.460	1.00	56.60	D
ATOM	7169	CG1	VAL	D	263	99.084	119.379	214.967	1.00	55.29	D
ATOM	7170	CG2	VAL	D	263	97.865	121.522	214.579	1.00	47.68	D
ATOM	7171	C	VAL	D	263	99.415	120.068	217.812	1.00	60.13	D
ATOM	7172	O	VAL	D	263	100.303	120.700	218.351	1.00	64.49	D
ATOM	7173	N	THR	D	264	99.299	118.761	217.959	1.00	58.39	D
ATOM	7174	CA	THR	D	264	100.209	118.044	218.827	1.00	59.70	D
ATOM	7175	CB	THR	D	264	99.541	117.866	220.169	1.00	56.54	D
ATOM	7176	OG1	THR	D	264	99.144	119.154	220.647	1.00	55.52	D
ATOM	7177	CG2	THR	D	264	100.457	117.185	221.155	1.00	46.38	D
ATOM	7178	C	THR	D	264	100.626	116.685	218.278	1.00	68.00	D
ATOM	7179	O	THR	D	264	99.837	115.995	217.634	1.00	72.49	D
ATOM	7180	N	ALA	D	265	101.869	116.297	218.539	1.00	71.03	D
ATOM	7181	CA	ALA	D	265	102.390	115.025	218.050	1.00	72.38	D
ATOM	7182	CB	ALA	D	265	103.833	114.855	218.482	1.00	75.56	D
ATOM	7183	C	ALA	D	265	101.574	113.834	218.521	1.00	73.65	D
ATOM	7184	O	ALA	D	265	100.883	113.899	219.540	1.00	75.04	D
ATOM	7185	N	GLY	D	266	101.669	112.742	217.764	1.00	74.97	D
ATOM	7186	CA	GLY	D	266	100.948	111.525	218.098	1.00	73.80	D
ATOM	7187	C	GLY	D	266	100.267	110.912	216.890	1.00	72.02	D
ATOM	7188	O	GLY	D	266	100.448	111.379	215.757	1.00	71.30	D
ATOM	7189	N	ASN	D	267	99.480	109.868	217.125	1.00	70.32	D
ATOM	7190	CA	ASN	D	267	98.766	109.206	216.039	1.00	69.49	D
ATOM	7191	CB	ASN	D	267	98.530	107.730	216.367	1.00	74.05	D
ATOM	7192	CG	ASN	D	267	99.776	106.891	216.191	1.00	78.81	D
ATOM	7193	OD1	ASN	D	267	99.751	105.672	216.367	1.00	77.68	D
ATOM	7194	ND2	ASN	D	267	100.877	107.540	215.835	1.00	80.93	D
ATOM	7195	C	ASN	D	267	97.428	109.862	215.700	1.00	65.66	D
ATOM	7196	O	ASN	D	267	96.789	110.499	216.541	1.00	59.57	D
ATOM	7197	N	VAL	D	268	97.028	109.703	214.443	1.00	62.93	D
ATOM	7198	CA	VAL	D	268	95.775	110.239	213.941	1.00	60.04	D
ATOM	7199	CB	VAL	D	268	96.008	111.435	213.003	1.00	59.12	D
ATOM	7200	CG1	VAL	D	268	94.683	111.936	212.454	1.00	59.32	D
ATOM	7201	CG2	VAL	D	268	96.706	112.545	213.757	1.00	64.04	D



ATOM	7202	C	VAL	D	268	95.096	109.121	213.165	1.00	59.11	D
ATOM	7203	O	VAL	D	268	95.550	108.724	212.094	1.00	57.26	D
ATOM	7204	N	GLN	D	269	94.022	108.595	213.733	1.00	59.62	D
ATOM	7205	CA	GLN	D	269	93.276	107.528	213.095	1.00	64.07	D
ATOM	7206	CB	GLN	D	269	93.407	106.245	213.916	1.00	66.32	D
ATOM	7207	CG	GLN	D	269	94.717	105.503	213.716	1.00	69.36	D
ATOM	7208	CD	GLN	D	269	94.900	104.367	214.711	1.00	75.58	D
ATOM	7209	OE1	GLN	D	269	93.992	103.567	214.938	1.00	78.64	D
ATOM	7210	NE2	GLN	D	269	96.087	104.286	215.304	1.00	79.82	D
ATOM	7211	C	GLN	D	269	91.806	107.925	212.939	1.00	66.74	D
ATOM	7212	O	GLN	D	269	91.286	108.750	213.697	1.00	67.92	D
ATOM	7213	N	SER	D	270	91.137	107.356	211.942	1.00	66.82	D
ATOM	7214	CA	SER	D	270	89.739	107.687	211.727	1.00	64.14	D
ATOM	7215	CB	SER	D	270	89.623	109.084	211.124	1.00	65.34	D
ATOM	7216	OG	SER	D	270	88.260	109.430	210.972	1.00	75.40	D
ATOM	7217	C	SER	D	270	88.961	106.697	210.870	1.00	61.93	D
ATOM	7218	O	SER	D	270	89.506	106.045	209.967	1.00	63.64	D
ATOM	7219	N	ILE	D	271	87.670	106.595	211.178	1.00	58.99	D
ATOM	7220	CA	ILE	D	271	86.746	105.706	210.480	1.00	53.49	D
ATOM	7221	CB	ILE	D	271	86.197	104.662	211.438	1.00	56.22	D
ATOM	7222	CG2	ILE	D	271	87.171	103.476	211.518	1.00	58.72	D
ATOM	7223	CG1	ILE	D	271	85.955	105.318	212.806	1.00	58.13	D
ATOM	7224	CD1	ILE	D	271	85.779	104.336	213.962	1.00	63.90	D
ATOM	7225	C	ILE	D	271	85.606	106.527	209.896	1.00	47.12	D
ATOM	7226	O	ILE	D	271	84.919	107.263	210.606	1.00	46.02	D
ATOM	7227	N	ILE	D	272	85.434	106.410	208.586	1.00	41.39	D
ATOM	7228	CA	ILE	D	272	84.411	107.145	207.869	1.00	36.85	D
ATOM	7229	CB	ILE	D	272	85.049	108.094	206.838	1.00	36.82	D
ATOM	7230	CG2	ILE	D	272	83.986	108.906	206.133	1.00	35.18	D
ATOM	7231	CG1	ILE	D	272	86.022	109.039	207.542	1.00	49.12	D
ATOM	7232	CD1	ILE	D	272	86.794	109.953	206.590	1.00	54.29	D
ATOM	7233	C	ILE	D	272	83.469	106.211	207.127	1.00	35.12	D
ATOM	7234	O	ILE	D	272	83.879	105.195	206.568	1.00	36.52	D
ATOM	7235	N	GLY	D	273	82.196	106.553	207.112	1.00	30.16	D
ATOM	7236	CA	GLY	D	273	81.279	105.719	206.382	1.00	31.96	D
ATOM	7237	C	GLY	D	273	80.998	106.344	205.039	1.00	34.87	D
ATOM	7238	O	GLY	D	273	80.799	107.568	204.941	1.00	33.97	D
ATOM	7239	N	VAL	D	274	81.028	105.514	203.996	1.00	33.38	D
ATOM	7240	CA	VAL	D	274	80.707	105.989	202.660	1.00	31.44	D
ATOM	7241	CB	VAL	D	274	81.816	105.679	201.627	1.00	30.80	D
ATOM	7242	CG1	VAL	D	274	81.595	106.540	200.375	1.00	23.78	D
ATOM	7243	CG2	VAL	D	274	83.183	105.971	202.212	1.00	28.59	D
ATOM	7244	C	VAL	D	274	79.436	105.244	202.282	1.00	31.51	D
ATOM	7245	O	VAL	D	274	79.434	104.021	202.172	1.00	30.40	D
ATOM	7246	N	THR	D	275	78.351	105.990	202.109	1.00	32.62	D
ATOM	7247	CA	THR	D	275	77.059	105.405	201.776	1.00	34.45	D
ATOM	7248	CB	THR	D	275	75.960	105.930	202.734	1.00	35.93	D
ATOM	7249	OG1	THR	D	275	76.209	105.430	204.047	1.00	37.09	D
ATOM	7250	CG2	THR	D	275	74.569	105.488	202.279	1.00	34.89	D
ATOM	7251	C	THR	D	275	76.610	105.679	200.351	1.00	32.81	D
ATOM	7252	O	THR	D	275	76.291	106.814	200.003	1.00	35.99	D
ATOM	7253	N	PHE	D	276	76.568	104.628	199.542	1.00	30.23	D
ATOM	7254	CA	PHE	D	276	76.126	104.744	198.163	1.00	29.91	D
ATOM	7255	CB	PHE	D	276	76.752	103.634	197.304	1.00	29.19	D
ATOM	7256	CG	PHE	D	276	78.209	103.834	197.041	1.00	31.68	D
ATOM	7257	CD1	PHE	D	276	79.158	103.451	197.979	1.00	29.72	D
ATOM	7258	CD2	PHE	D	276	78.634	104.475	195.876	1.00	35.46	D
ATOM	7259	CE1	PHE	D	276	80.519	103.704	197.764	1.00	34.64	D



ATOM	7260	CE2	PHE	D	276	79.997	104.737	195.648	1.00	32.43	D
ATOM	7261	CZ	PHE	D	276	80.939	104.350	196.593	1.00	31.28	D
ATOM	7262	C	PHE	D	276	74.607	104.656	198.111	1.00	28.75	D
ATOM	7263	O	PHE	D	276	74.021	103.683	198.568	1.00	28.84	D
ATOM	7264	N	VAL	D	277	73.970	105.678	197.557	1.00	28.81	D
ATOM	7265	CA	VAL	D	277	72.521	105.683	197.465	1.00	31.28	D
ATOM	7266	CB	VAL	D	277	71.952	107.063	197.763	1.00	33.59	D
ATOM	7267	CG1	VAL	D	277	70.446	106.970	197.865	1.00	29.66	D
ATOM	7268	CG2	VAL	D	277	72.555	107.600	199.056	1.00	31.85	D
ATOM	7269	C	VAL	D	277	72.031	105.262	196.094	1.00	30.61	D
ATOM	7270	O	VAL	D	277	72.436	105.835	195.088	1.00	30.84	D
ATOM	7271	N	TYR	D	278	71.148	104.264	196.074	1.00	28.20	D
ATOM	7272	CA	TYR	D	278	70.595	103.729	194.836	1.00	25.49	D
ATOM	7273	CB	TYR	D	278	70.412	102.223	194.941	1.00	24.29	D
ATOM	7274	CG	TYR	D	278	71.717	101.486	195.008	1.00	23.28	D
ATOM	7275	CD1	TYR	D	278	72.489	101.518	196.164	1.00	14.76	D
ATOM	7276	CE1	TYR	D	278	73.731	100.856	196.224	1.00	25.52	D
ATOM	7277	CD2	TYR	D	278	72.202	100.778	193.898	1.00	14.90	D
ATOM	7278	CE2	TYR	D	278	73.437	100.114	193.951	1.00	25.25	D
ATOM	7279	CZ	TYR	D	278	74.198	100.158	195.125	1.00	26.04	D
ATOM	7280	OH	TYR	D	278	75.404	99.492	195.219	1.00	29.19	D
ATOM	7281	C	TYR	D	278	69.288	104.329	194.419	1.00	26.91	D
ATOM	7282	O	TYR	D	278	68.370	104.474	195.229	1.00	26.77	D
ATOM	7283	N	GLN	D	279	69.203	104.678	193.141	1.00	27.38	D
ATOM	7284	CA	GLN	D	279	67.975	105.254	192.614	1.00	30.20	D
ATOM	7285	CB	GLN	D	279	68.261	106.005	191.314	1.00	24.11	D
ATOM	7286	CG	GLN	D	279	67.018	106.689	190.760	1.00	32.89	D
ATOM	7287	CD	GLN	D	279	67.189	107.256	189.349	1.00	39.19	D
ATOM	7288	OE1	GLN	D	279	66.406	108.117	188.937	1.00	40.33	D
ATOM	7289	NE2	GLN	D	279	68.194	106.765	188.599	1.00	31.57	D
ATOM	7290	C	GLN	D	279	66.861	104.198	192.399	1.00	30.38	D
ATOM	7291	O	GLN	D	279	65.694	104.508	192.721	1.00	32.03	D
ATOM	7292	OXT	GLN	D	279	67.153	103.081	191.908	1.00	26.20	D
ATOM	7293	C	GLY	E	1	55.769	44.624	90.619	1.00	46.04	E
ATOM	7294	O	GLY	E	1	55.952	45.783	90.252	1.00	50.74	E
ATOM	7295	N	GLY	E	1	53.461	44.241	91.215	1.00	45.11	E
ATOM	7296	CA	GLY	E	1	54.504	43.902	90.220	1.00	46.37	E
ATOM	7297	N	VAL	E	2	56.623	43.968	91.400	1.00	39.60	E
ATOM	7298	CA	VAL	E	2	57.867	44.585	91.829	1.00	34.00	E
ATOM	7299	CB	VAL	E	2	58.076	44.429	93.343	1.00	31.98	E
ATOM	7300	CG1	VAL	E	2	59.460	44.903	93.709	1.00	31.97	E
ATOM	7301	CG2	VAL	E	2	57.027	45.238	94.107	1.00	26.73	E
ATOM	7302	C	VAL	E	2	59.020	43.942	91.071	1.00	35.29	E
ATOM	7303	O	VAL	E	2	59.137	42.717	91.031	1.00	36.08	E
ATOM	7304	N	ALA	E	3	59.867	44.768	90.456	1.00	37.12	E
ATOM	7305	CA	ALA	E	3	60.986	44.245	89.676	1.00	36.47	E
ATOM	7306	CB	ALA	E	3	60.682	44.369	88.196	1.00	31.95	E
ATOM	7307	C	ALA	E	3	62.341	44.858	89.967	1.00	32.99	E
ATOM	7308	O	ALA	E	3	62.452	46.044	90.240	1.00	35.07	E
ATOM	7309	N	LEU	E	4	63.371	44.022	89.914	1.00	30.17	E
ATOM	7310	CA	LEU	E	4	64.722	44.478	90.140	1.00	28.06	E
ATOM	7311	CB	LEU	E	4	65.619	43.318	90.549	1.00	28.97	E
ATOM	7312	CG	LEU	E	4	65.232	42.571	91.821	1.00	27.63	E
ATOM	7313	CD1	LEU	E	4	66.355	41.613	92.198	1.00	26.09	E
ATOM	7314	CD2	LEU	E	4	64.965	43.554	92.922	1.00	26.55	E
ATOM	7315	C	LEU	E	4	65.223	45.061	88.834	1.00	31.45	E
ATOM	7316	O	LEU	E	4	64.792	44.630	87.751	1.00	33.65	E
ATOM	7317	N	GLY	E	5	66.138	46.028	88.940	1.00	31.71	E



ATOM	7318	CA	GLY	E	5	66.703	46.684	87.769	1.00	25.92	E
ATOM	7319	C	GLY	E	5	67.869	45.965	87.127	1.00	29.26	E
ATOM	7320	O	GLY	E	5	68.437	46.468	86.172	1.00	37.48	E
ATOM	7321	N	ALA	E	6	68.243	44.799	87.642	1.00	29.73	E
ATOM	7322	CA	ALA	E	6	69.341	44.019	87.066	1.00	30.56	E
ATOM	7323	CB	ALA	E	6	70.645	44.382	87.727	1.00	26.38	E
ATOM	7324	C	ALA	E	6	69.054	42.542	87.290	1.00	30.19	E
ATOM	7325	O	ALA	E	6	68.268	42.193	88.166	1.00	37.51	E
ATOM	7326	N	THR	E	7	69.685	41.676	86.516	1.00	22.98	E
ATOM	7327	CA	THR	E	7	69.474	40.255	86.681	1.00	21.43	E
ATOM	7328	CB	THR	E	7	69.254	39.549	85.328	1.00	20.53	E
ATOM	7329	OG1	THR	E	7	70.477	39.552	84.564	1.00	9.76	E
ATOM	7330	CG2	THR	E	7	68.115	40.242	84.554	1.00	15.59	E
ATOM	7331	C	THR	E	7	70.680	39.646	87.362	1.00	26.69	E
ATOM	7332	O	THR	E	7	70.826	38.424	87.416	1.00	28.87	E
ATOM	7333	N	ARG	E	8	71.553	40.510	87.869	1.00	28.25	E
ATOM	7334	CA	ARG	E	8	72.763	40.085	88.575	1.00	26.99	E
ATOM	7335	CB	ARG	E	8	73.712	39.314	87.670	1.00	24.88	E
ATOM	7336	CG	ARG	E	8	74.538	40.195	86.746	1.00	26.80	E
ATOM	7337	CD	ARG	E	8	74.293	39.869	85.288	1.00	27.21	E
ATOM	7338	NE	ARG	E	8	74.601	38.471	84.976	1.00	26.77	E
ATOM	7339	CZ	ARG	E	8	73.680	37.536	84.766	1.00	24.81	E
ATOM	7340	NH1	ARG	E	8	74.049	36.293	84.492	1.00	25.63	E
ATOM	7341	NH2	ARG	E	8	72.392	37.849	84.817	1.00	16.62	E
ATOM	7342	C	ARG	E	8	73.485	41.324	89.088	1.00	29.87	E
ATOM	7343	O	ARG	E	8	73.184	42.455	88.702	1.00	30.03	E
ATOM	7344	N	VAL	E	9	74.446	41.101	89.966	1.00	29.93	E
ATOM	7345	CA	VAL	E	9	75.184	42.188	90.555	1.00	27.67	E
ATOM	7346	CB	VAL	E	9	74.623	42.528	91.925	1.00	22.00	E
ATOM	7347	CG1	VAL	E	9	75.524	43.482	92.628	1.00	29.04	E
ATOM	7348	CG2	VAL	E	9	73.262	43.132	91.772	1.00	24.03	E
ATOM	7349	C	VAL	E	9	76.633	41.783	90.696	1.00	30.88	E
ATOM	7350	O	VAL	E	9	76.950	40.651	91.074	1.00	29.33	E
ATOM	7351	N	ILE	E	10	77.509	42.716	90.350	1.00	30.84	E
ATOM	7352	CA	ILE	E	10	78.929	42.495	90.461	1.00	31.61	E
ATOM	7353	CB	ILE	E	10	79.659	42.901	89.193	1.00	28.55	E
ATOM	7354	CG2	ILE	E	10	81.153	42.678	89.361	1.00	27.36	E
ATOM	7355	CG1	ILE	E	10	79.160	42.044	88.038	1.00	26.74	E
ATOM	7356	CD1	ILE	E	10	79.449	40.568	88.194	1.00	25.91	E
ATOM	7357	C	ILE	E	10	79.404	43.353	91.600	1.00	33.90	E
ATOM	7358	O	ILE	E	10	79.274	44.570	91.560	1.00	33.77	E
ATOM	7359	N	TYR	E	11	79.923	42.714	92.637	1.00	36.13	E
ATOM	7360	CA	TYR	E	11	80.417	43.458	93.781	1.00	37.06	E
ATOM	7361	CB	TYR	E	11	80.042	42.771	95.084	1.00	34.71	E
ATOM	7362	CG	TYR	E	11	80.051	43.713	96.257	1.00	39.58	E
ATOM	7363	CD1	TYR	E	11	78.883	44.356	96.659	1.00	41.57	E
ATOM	7364	CE1	TYR	E	11	78.879	45.263	97.711	1.00	38.13	E
ATOM	7365	CD2	TYR	E	11	81.226	44.001	96.943	1.00	37.32	E
ATOM	7366	CE2	TYR	E	11	81.230	44.915	98.000	1.00	38.53	E
ATOM	7367	CZ	TYR	E	11	80.049	45.542	98.375	1.00	36.39	E
ATOM	7368	OH	TYR	E	11	80.027	46.461	99.400	1.00	36.19	E
ATOM	7369	C	TYR	E	11	81.929	43.513	93.671	1.00	35.65	E
ATOM	7370	O	TYR	E	11	82.597	42.501	93.845	1.00	31.63	E
ATOM	7371	N	PRO	E	12	82.484	44.700	93.358	1.00	39.24	E
ATOM	7372	CD	PRO	E	12	81.743	45.915	92.978	1.00	41.90	E
ATOM	7373	CA	PRO	E	12	83.930	44.919	93.218	1.00	37.68	E
ATOM	7374	CB	PRO	E	12	84.019	46.312	92.605	1.00	35.89	E
ATOM	7375	CG	PRO	E	12	82.662	46.525	91.973	1.00	37.15	E



ATOM	7376	C	PRO	E	12	84.574	44.889	94.586	1.00	37.82	E
ATOM	7377	O	PRO	E	12	84.223	45.699	95.448	1.00	35.40	E
ATOM	7378	N	ALA	E	13	85.499	43.958	94.801	1.00	40.96	E
ATOM	7379	CA	ALA	E	13	86.162	43.877	96.093	1.00	45.60	E
ATOM	7380	CB	ALA	E	13	87.251	42.830	96.056	1.00	49.79	E
ATOM	7381	C	ALA	E	13	86.744	45.248	96.439	1.00	49.32	E
ATOM	7382	O	ALA	E	13	87.463	45.853	95.639	1.00	50.92	E
ATOM	7383	N	GLY	E	14	86.407	45.745	97.625	1.00	51.38	E
ATOM	7384	CA	GLY	E	14	86.901	47.041	98.038	1.00	51.83	E
ATOM	7385	C	GLY	E	14	85.792	48.065	98.146	1.00	55.57	E
ATOM	7386	O	GLY	E	14	85.746	48.817	99.118	1.00	56.03	E
ATOM	7387	N	GLN	E	15	84.903	48.101	97.154	1.00	57.81	E
ATOM	7388	CA	GLN	E	15	83.793	49.050	97.150	1.00	58.83	E
ATOM	7389	CB	GLN	E	15	82.776	48.685	96.067	1.00	62.35	E
ATOM	7390	CG	GLN	E	15	83.354	48.547	94.670	1.00	68.58	E
ATOM	7391	CD	GLN	E	15	83.252	49.815	93.843	1.00	71.63	E
ATOM	7392	OE1	GLN	E	15	83.691	50.887	94.262	1.00	74.06	E
ATOM	7393	NE2	GLN	E	15	82.673	49.695	92.651	1.00	74.53	E
ATOM	7394	C	GLN	E	15	83.107	49.024	98.504	1.00	60.94	E
ATOM	7395	O	GLN	E	15	82.876	47.963	99.077	1.00	61.51	E
ATOM	7396	N	LYS	E	16	82.784	50.193	99.027	1.00	63.19	E
ATOM	7397	CA	LYS	E	16	82.121	50.245	100.312	1.00	66.63	E
ATOM	7398	CB	LYS	E	16	82.074	51.681	100.822	1.00	73.67	E
ATOM	7399	CG	LYS	E	16	81.574	51.819	102.254	1.00	80.94	E
ATOM	7400	CD	LYS	E	16	81.362	53.286	102.642	1.00	87.89	E
ATOM	7401	CE	LYS	E	16	82.528	54.182	102.190	1.00	90.92	E
ATOM	7402	NZ	LYS	E	16	83.861	53.711	102.676	1.00	94.46	E
ATOM	7403	C	LYS	E	16	80.703	49.718	100.152	1.00	67.02	E
ATOM	7404	O	LYS	E	16	80.126	49.175	101.092	1.00	70.07	E
ATOM	7405	N	GLN	E	17	80.147	49.869	98.952	1.00	64.08	E
ATOM	7406	CA	GLN	E	17	78.781	49.426	98.692	1.00	60.31	E
ATOM	7407	CB	GLN	E	17	77.808	50.268	99.514	1.00	59.69	E
ATOM	7408	CG	GLN	E	17	77.955	51.732	99.224	1.00	61.22	E
ATOM	7409	CD	GLN	E	17	76.698	52.513	99.493	1.00	65.20	E
ATOM	7410	OE1	GLN	E	17	76.180	52.519	100.622	1.00	64.50	E
ATOM	7411	NE2	GLN	E	17	76.194	53.197	98.453	1.00	58.46	E
ATOM	7412	C	GLN	E	17	78.361	49.517	97.226	1.00	54.80	E
ATOM	7413	O	GLN	E	17	78.794	50.403	96.502	1.00	57.05	E
ATOM	7414	N	VAL	E	18	77.504	48.595	96.802	1.00	48.39	E
ATOM	7415	CA	VAL	E	18	76.998	48.593	95.444	1.00	44.30	E
ATOM	7416	CB	VAL	E	18	77.286	47.278	94.738	1.00	44.09	E
ATOM	7417	CG1	VAL	E	18	76.675	47.290	93.351	1.00	43.03	E
ATOM	7418	CG2	VAL	E	18	78.780	47.072	94.641	1.00	49.03	E
ATOM	7419	C	VAL	E	18	75.499	48.782	95.560	1.00	45.32	E
ATOM	7420	O	VAL	E	18	74.898	48.408	96.563	1.00	48.67	E
ATOM	7421	N	GLN	E	19	74.886	49.376	94.550	1.00	42.05	E
ATOM	7422	CA	GLN	E	19	73.465	49.596	94.625	1.00	41.76	E
ATOM	7423	CB	GLN	E	19	73.185	51.083	94.727	1.00	44.42	E
ATOM	7424	CG	GLN	E	19	73.948	51.916	93.749	1.00	53.82	E
ATOM	7425	CD	GLN	E	19	74.034	53.358	94.192	1.00	56.57	E
ATOM	7426	OE1	GLN	E	19	74.652	53.665	95.209	1.00	59.10	E
ATOM	7427	NE2	GLN	E	19	73.404	54.253	93.437	1.00	62.38	E
ATOM	7428	C	GLN	E	19	72.681	48.966	93.491	1.00	39.95	E
ATOM	7429	O	GLN	E	19	73.177	48.829	92.385	1.00	38.80	E
ATOM	7430	N	LEU	E	20	71.455	48.563	93.812	1.00	36.92	E
ATOM	7431	CA	LEU	E	20	70.542	47.910	92.891	1.00	34.38	E
ATOM	7432	CB	LEU	E	20	70.337	46.457	93.336	1.00	33.96	E
ATOM	7433	CG	LEU	E	20	69.434	45.520	92.521	1.00	37.59	E



ATOM	7434	CD1	LEU	E	20	70.071	45.233	91.176	1.00	30.23	E
ATOM	7435	CD2	LEU	E	20	69.227	44.219	93.278	1.00	34.96	E
ATOM	7436	C	LEU	E	20	69.208	48.668	92.912	1.00	35.04	E
ATOM	7437	O	LEU	E	20	68.804	49.205	93.942	1.00	34.98	E
ATOM	7438	N	ALA	E	21	68.525	48.708	91.776	1.00	34.62	E
ATOM	7439	CA	ALA	E	21	67.264	49.424	91.692	1.00	32.72	E
ATOM	7440	CB	ALA	E	21	67.174	50.184	90.375	1.00	28.04	E
ATOM	7441	C	ALA	E	21	66.094	48.487	91.804	1.00	34.50	E
ATOM	7442	O	ALA	E	21	66.149	47.342	91.351	1.00	33.01	E
ATOM	7443	N	VAL	E	22	65.031	48.997	92.410	1.00	36.31	E
ATOM	7444	CA	VAL	E	22	63.807	48.249	92.580	1.00	38.07	E
ATOM	7445	CB	VAL	E	22	63.502	47.893	94.036	1.00	39.99	E
ATOM	7446	CG1	VAL	E	22	62.715	46.594	94.085	1.00	34.81	E
ATOM	7447	CG2	VAL	E	22	64.765	47.819	94.829	1.00	40.01	E
ATOM	7448	C	VAL	E	22	62.733	49.207	92.176	1.00	41.59	E
ATOM	7449	O	VAL	E	22	62.753	50.384	92.552	1.00	42.62	E
ATOM	7450	N	THR	E	23	61.773	48.690	91.436	1.00	43.32	E
ATOM	7451	CA	THR	E	23	60.679	49.502	90.988	1.00	45.01	E
ATOM	7452	CB	THR	E	23	60.913	49.923	89.539	1.00	46.09	E
ATOM	7453	OG1	THR	E	23	59.680	50.362	88.967	1.00	56.87	E
ATOM	7454	CG2	THR	E	23	61.466	48.769	88.737	1.00	51.13	E
ATOM	7455	C	THR	E	23	59.396	48.696	91.134	1.00	44.67	E
ATOM	7456	O	THR	E	23	59.370	47.503	90.852	1.00	41.77	E
ATOM	7457	N	ASN	E	24	58.348	49.369	91.603	1.00	47.65	E
ATOM	7458	CA	ASN	E	24	57.034	48.782	91.820	1.00	46.62	E
ATOM	7459	CB	ASN	E	24	56.557	49.126	93.232	1.00	44.81	E
ATOM	7460	CG	ASN	E	24	55.112	48.716	93.484	1.00	50.55	E
ATOM	7461	OD1	ASN	E	24	54.589	47.823	92.820	1.00	48.83	E
ATOM	7462	ND2	ASN	E	24	54.469	49.357	94.462	1.00	47.77	E
ATOM	7463	C	ASN	E	24	56.059	49.334	90.786	1.00	51.07	E
ATOM	7464	O	ASN	E	24	55.732	50.526	90.801	1.00	51.24	E
ATOM	7465	N	ASN	E	25	55.608	48.452	89.895	1.00	54.60	E
ATOM	7466	CA	ASN	E	25	54.672	48.783	88.811	1.00	58.05	E
ATOM	7467	CB	ASN	E	25	54.582	47.628	87.815	1.00	55.36	E
ATOM	7468	CG	ASN	E	25	55.878	47.372	87.106	1.00	55.70	E
ATOM	7469	OD1	ASN	E	25	56.959	47.607	87.650	1.00	53.11	E
ATOM	7470	ND2	ASN	E	25	55.785	46.862	85.887	1.00	59.68	E
ATOM	7471	C	ASN	E	25	53.260	49.069	89.285	1.00	61.01	E
ATOM	7472	O	ASN	E	25	52.685	50.110	88.985	1.00	64.11	E
ATOM	7473	N	ASP	E	26	52.699	48.111	90.006	1.00	61.50	E
ATOM	7474	CA	ASP	E	26	51.346	48.216	90.508	1.00	63.45	E
ATOM	7475	CB	ASP	E	26	51.132	47.189	91.603	1.00	67.89	E
ATOM	7476	CG	ASP	E	26	51.287	45.776	91.098	1.00	67.98	E
ATOM	7477	OD1	ASP	E	26	51.186	44.850	91.929	1.00	67.86	E
ATOM	7478	OD2	ASP	E	26	51.510	45.598	89.875	1.00	68.04	E
ATOM	7479	C	ASP	E	26	50.946	49.584	91.007	1.00	63.91	E
ATOM	7480	O	ASP	E	26	51.202	49.947	92.150	1.00	62.99	E
ATOM	7481	N	GLU	E	27	50.289	50.325	90.128	1.00	67.19	E
ATOM	7482	CA	GLU	E	27	49.822	51.668	90.422	1.00	70.83	E
ATOM	7483	CB	GLU	E	27	48.886	52.136	89.300	1.00	75.40	E
ATOM	7484	CG	GLU	E	27	49.647	52.567	88.037	1.00	88.94	E
ATOM	7485	CD	GLU	E	27	48.897	52.306	86.733	1.00	93.88	E
ATOM	7486	OE1	GLU	E	27	47.719	52.720	86.620	1.00	99.08	E
ATOM	7487	OE2	GLU	E	27	49.498	51.695	85.818	1.00	94.17	E
ATOM	7488	C	GLU	E	27	49.134	51.788	91.771	1.00	69.46	E
ATOM	7489	O	GLU	E	27	49.069	52.875	92.331	1.00	68.88	E
ATOM	7490	N	ASN	E	28	48.635	50.684	92.310	1.00	69.07	E
ATOM	7491	CA	ASN	E	28	47.959	50.770	93.591	1.00	71.81	E



ATOM	7492	CB	ASN	E	28	46.517	51.256	93.381	1.00	77.74	E
ATOM	7493	CG	ASN	E	28	45.772	50.452	92.323	1.00	80.56	E
ATOM	7494	OD1	ASN	E	28	44.694	50.850	91.874	1.00	79.29	E
ATOM	7495	ND2	ASN	E	28	46.343	49.317	91.921	1.00	81.29	E
ATOM	7496	C	ASN	E	28	47.976	49.487	94.399	1.00	71.02	E
ATOM	7497	O	ASN	E	28	47.183	48.582	94.175	1.00	74.33	E
ATOM	7498	N	SER	E	29	48.889	49.441	95.357	1.00	70.27	E
ATOM	7499	CA	SER	E	29	49.085	48.302	96.244	1.00	68.04	E
ATOM	7500	CB	SER	E	29	49.056	46.983	95.460	1.00	70.30	E
ATOM	7501	OG	SER	E	29	50.068	46.950	94.465	1.00	72.13	E
ATOM	7502	C	SER	E	29	50.461	48.501	96.872	1.00	64.52	E
ATOM	7503	O	SER	E	29	51.471	48.521	96.173	1.00	65.38	E
ATOM	7504	N	THR	E	30	50.503	48.668	98.185	1.00	60.80	E
ATOM	7505	CA	THR	E	30	51.776	48.878	98.848	1.00	58.83	E
ATOM	7506	CB	THR	E	30	51.577	49.543	100.215	1.00	59.00	E
ATOM	7507	OG1	THR	E	30	50.777	50.721	100.060	1.00	63.07	E
ATOM	7508	CG2	THR	E	30	52.902	49.958	100.794	1.00	64.32	E
ATOM	7509	C	THR	E	30	52.502	47.554	99.027	1.00	54.38	E
ATOM	7510	O	THR	E	30	51.896	46.491	98.950	1.00	56.36	E
ATOM	7511	N	TYR	E	31	53.808	47.625	99.242	1.00	50.30	E
ATOM	7512	CA	TYR	E	31	54.620	46.431	99.447	1.00	48.42	E
ATOM	7513	CB	TYR	E	31	55.301	46.004	98.158	1.00	46.28	E
ATOM	7514	CG	TYR	E	31	54.409	45.324	97.168	1.00	48.73	E
ATOM	7515	CD1	TYR	E	31	54.081	45.936	95.957	1.00	48.25	E
ATOM	7516	CE1	TYR	E	31	53.325	45.269	95.007	1.00	52.85	E
ATOM	7517	CD2	TYR	E	31	53.950	44.033	97.401	1.00	51.20	E
ATOM	7518	CE2	TYR	E	31	53.194	43.354	96.452	1.00	51.10	E
ATOM	7519	CZ	TYR	E	31	52.888	43.975	95.261	1.00	53.18	E
ATOM	7520	OH	TYR	E	31	52.169	43.287	94.316	1.00	60.86	E
ATOM	7521	C	TYR	E	31	55.714	46.675	100.474	1.00	47.23	E
ATOM	7522	O	TYR	E	31	56.178	47.799	100.673	1.00	48.94	E
ATOM	7523	N	LEU	E	32	56.116	45.609	101.141	1.00	43.24	E
ATOM	7524	CA	LEU	E	32	57.188	45.698	102.103	1.00	41.02	E
ATOM	7525	CB	LEU	E	32	56.831	44.969	103.394	1.00	48.09	E
ATOM	7526	CG	LEU	E	32	56.084	45.770	104.452	1.00	48.22	E
ATOM	7527	CD1	LEU	E	32	55.647	44.834	105.573	1.00	51.45	E
ATOM	7528	CD2	LEU	E	32	56.985	46.881	104.969	1.00	45.46	E
ATOM	7529	C	LEU	E	32	58.332	44.988	101.414	1.00	41.92	E
ATOM	7530	O	LEU	E	32	58.222	43.812	101.025	1.00	37.70	E
ATOM	7531	N	ILE	E	33	59.420	45.715	101.229	1.00	37.61	E
ATOM	7532	CA	ILE	E	33	60.576	45.146	100.590	1.00	34.91	E
ATOM	7533	CB	ILE	E	33	61.274	46.201	99.735	1.00	36.77	E
ATOM	7534	CG2	ILE	E	33	62.455	45.589	98.986	1.00	35.38	E
ATOM	7535	CG1	ILE	E	33	60.248	46.828	98.786	1.00	35.93	E
ATOM	7536	CD1	ILE	E	33	59.432	45.825	97.997	1.00	27.30	E
ATOM	7537	C	ILE	E	33	61.506	44.649	101.677	1.00	36.05	E
ATOM	7538	O	ILE	E	33	61.890	45.395	102.580	1.00	37.16	E
ATOM	7539	N	GLN	E	34	61.848	43.376	101.590	1.00	36.50	E
ATOM	7540	CA	GLN	E	34	62.736	42.746	102.553	1.00	38.13	E
ATOM	7541	CB	GLN	E	34	61.952	41.723	103.364	1.00	42.99	E
ATOM	7542	CG	GLN	E	34	62.462	41.486	104.751	1.00	43.07	E
ATOM	7543	CD	GLN	E	34	61.560	40.559	105.516	1.00	45.87	E
ATOM	7544	OE1	GLN	E	34	61.405	39.390	105.157	1.00	50.95	E
ATOM	7545	NE2	GLN	E	34	60.943	41.074	106.571	1.00	45.05	E
ATOM	7546	C	GLN	E	34	63.806	42.048	101.722	1.00	36.62	E
ATOM	7547	O	GLN	E	34	63.508	41.128	100.971	1.00	35.14	E
ATOM	7548	N	SER	E	35	65.050	42.483	101.862	1.00	36.66	E
ATOM	7549	CA	SER	E	35	66.138	41.910	101.083	1.00	37.23	E



ATOM	7550	CB	SER	E	35	66.759	43.006	100.221	1.00	40.58	E
ATOM	7551	OG	SER	E	35	65.744	43.789	99.628	1.00	52.81	E
ATOM	7552	C	SER	E	35	67.231	41.263	101.919	1.00	34.80	E
ATOM	7553	O	SER	E	35	67.469	41.652	103.055	1.00	40.19	E
ATOM	7554	N	TRP	E	36	67.899	40.274	101.347	1.00	29.82	E
ATOM	7555	CA	TRP	E	36	69.004	39.611	102.026	1.00	30.01	E
ATOM	7556	CB	TRP	E	36	68.500	38.630	103.074	1.00	19.84	E
ATOM	7557	CG	TRP	E	36	67.917	37.385	102.516	1.00	24.65	E
ATOM	7558	CD2	TRP	E	36	66.571	37.200	102.068	1.00	21.26	E
ATOM	7559	CE2	TRP	E	36	66.466	35.871	101.597	1.00	26.04	E
ATOM	7560	CE3	TRP	E	36	65.443	38.026	102.024	1.00	19.55	E
ATOM	7561	CD1	TRP	E	36	68.560	36.199	102.306	1.00	25.27	E
ATOM	7562	NE1	TRP	E	36	67.695	35.283	101.753	1.00	27.64	E
ATOM	7563	CZ2	TRP	E	36	65.269	35.346	101.084	1.00	21.61	E
ATOM	7564	CZ3	TRP	E	36	64.243	37.506	101.517	1.00	18.87	E
ATOM	7565	CH2	TRP	E	36	64.170	36.175	101.055	1.00	21.25	E
ATOM	7566	C	TRP	E	36	69.891	38.885	101.017	1.00	29.36	E
ATOM	7567	O	TRP	E	36	69.573	38.787	99.833	1.00	29.46	E
ATOM	7568	N	VAL	E	37	71.009	38.377	101.495	1.00	27.63	E
ATOM	7569	CA	VAL	E	37	71.923	37.697	100.622	1.00	28.21	E
ATOM	7570	CB	VAL	E	37	73.158	38.574	100.344	1.00	29.01	E
ATOM	7571	CG1	VAL	E	37	74.122	37.842	99.439	1.00	30.04	E
ATOM	7572	CG2	VAL	E	37	72.724	39.869	99.707	1.00	25.95	E
ATOM	7573	C	VAL	E	37	72.362	36.409	101.267	1.00	28.25	E
ATOM	7574	O	VAL	E	37	72.847	36.405	102.393	1.00	33.23	E
ATOM	7575	N	GLU	E	38	72.178	35.315	100.547	1.00	26.36	E
ATOM	7576	CA	GLU	E	38	72.584	34.011	101.031	1.00	28.53	E
ATOM	7577	CB	GLU	E	38	71.531	32.975	100.670	1.00	24.91	E
ATOM	7578	CG	GLU	E	38	70.183	33.306	101.281	1.00	33.69	E
ATOM	7579	CD	GLU	E	38	69.091	32.454	100.729	1.00	33.38	E
ATOM	7580	OE1	GLU	E	38	69.453	31.398	100.158	1.00	31.38	E
ATOM	7581	OE2	GLU	E	38	67.894	32.833	100.867	1.00	28.30	E
ATOM	7582	C	GLU	E	38	73.884	33.707	100.328	1.00	30.16	E
ATOM	7583	O	GLU	E	38	74.184	34.307	99.295	1.00	32.61	E
ATOM	7584	N	ASN	E	39	74.679	32.810	100.895	1.00	30.97	E
ATOM	7585	CA	ASN	E	39	75.930	32.456	100.254	1.00	30.12	E
ATOM	7586	CB	ASN	E	39	76.990	32.038	101.273	1.00	30.70	E
ATOM	7587	CG	ASN	E	39	76.626	30.768	102.021	1.00	39.43	E
ATOM	7588	OD1	ASN	E	39	75.807	29.965	101.566	1.00	42.90	E
ATOM	7589	ND2	ASN	E	39	77.253	30.571	103.171	1.00	40.16	E
ATOM	7590	C	ASN	E	39	75.642	31.315	99.291	1.00	30.88	E
ATOM	7591	O	ASN	E	39	74.488	30.902	99.138	1.00	24.86	E
ATOM	7592	N	ALA	E	40	76.695	30.811	98.651	1.00	32.96	E
ATOM	7593	CA	ALA	E	40	76.569	29.745	97.674	1.00	33.48	E
ATOM	7594	CB	ALA	E	40	77.923	29.317	97.220	1.00	35.60	E
ATOM	7595	C	ALA	E	40	75.794	28.552	98.193	1.00	37.35	E
ATOM	7596	O	ALA	E	40	75.035	27.939	97.458	1.00	38.58	E
ATOM	7597	N	ASP	E	41	75.974	28.212	99.459	1.00	39.62	E
ATOM	7598	CA	ASP	E	41	75.258	27.076	99.995	1.00	43.38	E
ATOM	7599	CB	ASP	E	41	75.998	26.507	101.191	1.00	47.76	E
ATOM	7600	CG	ASP	E	41	77.280	25.822	100.792	1.00	50.10	E
ATOM	7601	OD1	ASP	E	41	77.233	24.996	99.856	1.00	50.92	E
ATOM	7602	OD2	ASP	E	41	78.325	26.104	101.416	1.00	50.93	E
ATOM	7603	C	ASP	E	41	73.818	27.373	100.369	1.00	45.89	E
ATOM	7604	O	ASP	E	41	73.110	26.496	100.849	1.00	51.61	E
ATOM	7605	N	GLY	E	42	73.379	28.602	100.146	1.00	43.17	E
ATOM	7606	CA	GLY	E	42	72.008	28.942	100.461	1.00	37.95	E
ATOM	7607	C	GLY	E	42	71.805	29.399	101.886	1.00	37.65	E



ATOM	7608	O	GLY	E	42	70.680	29.692	102.277	1.00	38.17	E
ATOM	7609	N	VAL	E	43	72.869	29.481	102.678	1.00	38.96	E
ATOM	7610	CA	VAL	E	43	72.687	29.914	104.055	1.00	39.36	E
ATOM	7611	CB	VAL	E	43	73.606	29.134	105.041	1.00	34.67	E
ATOM	7612	CG1	VAL	E	43	74.302	28.008	104.334	1.00	32.49	E
ATOM	7613	CG2	VAL	E	43	74.590	30.061	105.701	1.00	39.40	E
ATOM	7614	C	VAL	E	43	72.874	31.418	104.229	1.00	41.65	E
ATOM	7615	O	VAL	E	43	73.755	32.028	103.611	1.00	41.79	E
ATOM	7616	N	LYS	E	44	72.022	32.005	105.068	1.00	40.31	E
ATOM	7617	CA	LYS	E	44	72.069	33.427	105.333	1.00	41.11	E
ATOM	7618	CB	LYS	E	44	70.749	33.912	105.945	1.00	41.89	E
ATOM	7619	CG	LYS	E	44	69.497	33.731	105.101	1.00	41.17	E
ATOM	7620	CD	LYS	E	44	68.484	32.872	105.826	1.00	45.18	E
ATOM	7621	CE	LYS	E	44	67.213	32.708	105.026	1.00	47.59	E
ATOM	7622	NZ	LYS	E	44	66.586	34.029	104.799	1.00	55.78	E
ATOM	7623	C	LYS	E	44	73.195	33.780	106.300	1.00	43.34	E
ATOM	7624	O	LYS	E	44	72.955	33.945	107.498	1.00	41.72	E
ATOM	7625	N	ASP	E	45	74.429	33.855	105.814	1.00	44.22	E
ATOM	7626	CA	ASP	E	45	75.496	34.281	106.703	1.00	43.51	E
ATOM	7627	CB	ASP	E	45	76.854	33.768	106.261	1.00	46.06	E
ATOM	7628	CG	ASP	E	45	77.064	33.884	104.780	1.00	45.99	E
ATOM	7629	OD1	ASP	E	45	76.505	34.822	104.171	1.00	48.45	E
ATOM	7630	OD2	ASP	E	45	77.805	33.041	104.239	1.00	35.15	E
ATOM	7631	C	ASP	E	45	75.418	35.778	106.547	1.00	45.51	E
ATOM	7632	O	ASP	E	45	74.549	36.282	105.825	1.00	50.35	E
ATOM	7633	N	GLY	E	46	76.308	36.511	107.183	1.00	45.87	E
ATOM	7634	CA	GLY	E	46	76.179	37.953	107.065	1.00	45.12	E
ATOM	7635	C	GLY	E	46	77.190	38.572	106.152	1.00	45.17	E
ATOM	7636	O	GLY	E	46	77.455	39.768	106.259	1.00	46.18	E
ATOM	7637	N	ARG	E	47	77.754	37.765	105.256	1.00	43.73	E
ATOM	7638	CA	ARG	E	47	78.761	38.258	104.338	1.00	40.06	E
ATOM	7639	CB	ARG	E	47	79.084	37.202	103.300	1.00	47.98	E
ATOM	7640	CG	ARG	E	47	80.439	36.575	103.522	1.00	58.67	E
ATOM	7641	CD	ARG	E	47	80.465	35.732	104.771	1.00	67.69	E
ATOM	7642	NE	ARG	E	47	81.817	35.259	105.047	1.00	78.50	E
ATOM	7643	CZ	ARG	E	47	82.764	36.007	105.606	1.00	86.38	E
ATOM	7644	NH1	ARG	E	47	82.498	37.258	105.954	1.00	90.89	E
ATOM	7645	NH2	ARG	E	47	83.978	35.511	105.816	1.00	91.15	E
ATOM	7646	C	ARG	E	47	78.350	39.554	103.663	1.00	39.17	E
ATOM	7647	O	ARG	E	47	79.172	40.443	103.450	1.00	38.55	E
ATOM	7648	N	PHE	E	48	77.075	39.677	103.332	1.00	37.09	E
ATOM	7649	CA	PHE	E	48	76.606	40.897	102.694	1.00	38.80	E
ATOM	7650	CB	PHE	E	48	76.395	40.685	101.181	1.00	36.91	E
ATOM	7651	CG	PHE	E	48	77.669	40.490	100.429	1.00	33.48	E
ATOM	7652	CD1	PHE	E	48	78.232	39.222	100.308	1.00	35.80	E
ATOM	7653	CD2	PHE	E	48	78.369	41.591	99.935	1.00	35.12	E
ATOM	7654	CE1	PHE	E	48	79.475	39.053	99.719	1.00	32.89	E
ATOM	7655	CE2	PHE	E	48	79.609	41.441	99.346	1.00	30.41	E
ATOM	7656	CZ	PHE	E	48	80.171	40.173	99.237	1.00	33.91	E
ATOM	7657	C	PHE	E	48	75.325	41.371	103.340	1.00	35.91	E
ATOM	7658	O	PHE	E	48	74.501	40.563	103.721	1.00	33.62	E
ATOM	7659	N	ILE	E	49	75.166	42.685	103.456	1.00	36.47	E
ATOM	7660	CA	ILE	E	49	73.978	43.251	104.061	1.00	38.80	E
ATOM	7661	CB	ILE	E	49	74.329	43.872	105.415	1.00	43.00	E
ATOM	7662	CG2	ILE	E	49	73.105	44.516	106.050	1.00	39.31	E
ATOM	7663	CG1	ILE	E	49	74.827	42.759	106.333	1.00	46.46	E
ATOM	7664	CD1	ILE	E	49	75.603	43.252	107.517	1.00	55.41	E
ATOM	7665	C	ILE	E	49	73.350	44.271	103.132	1.00	36.76	E



ATOM	7666	O	ILE	E	49	74.036	45.066	102.503	1.00	39.20	E
ATOM	7667	N	VAL	E	50	72.032	44.239	103.046	1.00	34.79	E
ATOM	7668	CA	VAL	E	50	71.317	45.134	102.160	1.00	37.93	E
ATOM	7669	CB	VAL	E	50	70.330	44.341	101.261	1.00	39.57	E
ATOM	7670	CG1	VAL	E	50	69.669	45.266	100.257	1.00	36.69	E
ATOM	7671	CG2	VAL	E	50	71.061	43.201	100.565	1.00	38.22	E
ATOM	7672	C	VAL	E	50	70.528	46.127	102.974	1.00	38.90	E
ATOM	7673	O	VAL	E	50	69.997	45.778	104.024	1.00	41.68	E
ATOM	7674	N	THR	E	51	70.453	47.364	102.501	1.00	38.15	E
ATOM	7675	CA	THR	E	51	69.677	48.382	103.201	1.00	36.56	E
ATOM	7676	CB	THR	E	51	70.551	49.391	103.965	1.00	40.10	E
ATOM	7677	OG1	THR	E	51	71.482	49.996	103.061	1.00	47.13	E
ATOM	7678	CG2	THR	E	51	71.301	48.717	105.092	1.00	47.78	E
ATOM	7679	C	THR	E	51	68.887	49.175	102.194	1.00	34.88	E
ATOM	7680	O	THR	E	51	69.318	49.367	101.062	1.00	38.30	E
ATOM	7681	N	PRO	E	52	67.692	49.606	102.578	1.00	33.42	E
ATOM	7682	CD	PRO	E	52	67.019	50.775	101.994	1.00	34.56	E
ATOM	7683	CA	PRO	E	52	67.163	49.313	103.909	1.00	34.06	E
ATOM	7684	CB	PRO	E	52	66.013	50.308	104.062	1.00	32.31	E
ATOM	7685	CG	PRO	E	52	65.688	50.716	102.659	1.00	38.55	E
ATOM	7686	C	PRO	E	52	66.690	47.873	103.994	1.00	34.91	E
ATOM	7687	O	PRO	E	52	66.071	47.360	103.071	1.00	39.18	E
ATOM	7688	N	PRO	E	53	66.981	47.197	105.104	1.00	31.85	E
ATOM	7689	CD	PRO	E	53	67.614	47.687	106.341	1.00	30.37	E
ATOM	7690	CA	PRO	E	53	66.552	45.808	105.244	1.00	29.51	E
ATOM	7691	CB	PRO	E	53	67.074	45.431	106.622	1.00	30.67	E
ATOM	7692	CG	PRO	E	53	67.043	46.759	107.368	1.00	25.10	E
ATOM	7693	C	PRO	E	53	65.044	45.603	105.127	1.00	30.54	E
ATOM	7694	O	PRO	E	53	64.589	44.497	104.861	1.00	29.65	E
ATOM	7695	N	LEU	E	54	64.269	46.666	105.326	1.00	33.04	E
ATOM	7696	CA	LEU	E	54	62.806	46.571	105.261	1.00	34.09	E
ATOM	7697	CB	LEU	E	54	62.259	46.017	106.564	1.00	34.21	E
ATOM	7698	CG	LEU	E	54	60.740	45.916	106.662	1.00	36.10	E
ATOM	7699	CD1	LEU	E	54	60.270	44.653	105.941	1.00	41.54	E
ATOM	7700	CD2	LEU	E	54	60.336	45.866	108.124	1.00	35.95	E
ATOM	7701	C	LEU	E	54	62.181	47.930	105.048	1.00	36.11	E
ATOM	7702	O	LEU	E	54	62.406	48.836	105.855	1.00	41.13	E
ATOM	7703	N	PHE	E	55	61.388	48.078	103.992	1.00	31.85	E
ATOM	7704	CA	PHE	E	55	60.758	49.365	103.709	1.00	34.55	E
ATOM	7705	CB	PHE	E	55	61.755	50.322	103.057	1.00	34.74	E
ATOM	7706	CG	PHE	E	55	62.247	49.857	101.725	1.00	41.52	E
ATOM	7707	CD1	PHE	E	55	61.644	50.294	100.551	1.00	46.13	E
ATOM	7708	CD2	PHE	E	55	63.296	48.950	101.641	1.00	43.23	E
ATOM	7709	CE1	PHE	E	55	62.084	49.832	99.300	1.00	46.53	E
ATOM	7710	CE2	PHE	E	55	63.740	48.485	100.407	1.00	49.59	E
ATOM	7711	CZ	PHE	E	55	63.134	48.925	99.231	1.00	48.47	E
ATOM	7712	C	PHE	E	55	59.565	49.205	102.801	1.00	37.80	E
ATOM	7713	O	PHE	E	55	59.388	48.158	102.164	1.00	39.42	E
ATOM	7714	N	ALA	E	56	58.747	50.252	102.732	1.00	41.26	E
ATOM	7715	CA	ALA	E	56	57.544	50.215	101.906	1.00	40.53	E
ATOM	7716	CB	ALA	E	56	56.368	50.739	102.700	1.00	36.38	E
ATOM	7717	C	ALA	E	56	57.640	50.957	100.574	1.00	39.61	E
ATOM	7718	O	ALA	E	56	58.326	51.971	100.437	1.00	40.56	E
ATOM	7719	N	MET	E	57	56.957	50.416	99.582	1.00	40.87	E
ATOM	7720	CA	MET	E	57	56.896	51.025	98.269	1.00	42.37	E
ATOM	7721	CB	MET	E	57	57.570	50.149	97.223	1.00	41.04	E
ATOM	7722	CG	MET	E	57	59.033	49.903	97.488	1.00	43.96	E
ATOM	7723	SD	MET	E	57	59.975	49.889	95.957	1.00	44.93	E



ATOM	7724	CE	MET	E	57	59.317	48.456	95.232	1.00	52.13	E
ATOM	7725	C	MET	E	57	55.406	51.139	97.986	1.00	44.69	E
ATOM	7726	O	MET	E	57	54.722	50.134	97.758	1.00	43.13	E
ATOM	7727	N	LYS	E	58	54.905	52.366	98.038	1.00	45.78	E
ATOM	7728	CA	LYS	E	58	53.496	52.614	97.803	1.00	53.73	E
ATOM	7729	CB	LYS	E	58	53.006	53.704	98.756	1.00	60.16	E
ATOM	7730	CG	LYS	E	58	51.500	53.755	98.917	1.00	66.91	E
ATOM	7731	CD	LYS	E	58	51.090	54.908	99.820	1.00	73.01	E
ATOM	7732	CE	LYS	E	58	49.734	54.648	100.470	1.00	77.37	E
ATOM	7733	NZ	LYS	E	58	49.784	53.487	101.417	1.00	74.60	E
ATOM	7734	C	LYS	E	58	53.222	53.022	96.355	1.00	54.93	E
ATOM	7735	O	LYS	E	58	53.727	54.038	95.877	1.00	57.77	E
ATOM	7736	N	GLY	E	59	52.415	52.225	95.662	1.00	54.84	E
ATOM	7737	CA	GLY	E	59	52.087	52.532	94.283	1.00	52.96	E
ATOM	7738	C	GLY	E	59	53.328	52.590	93.421	1.00	51.28	E
ATOM	7739	O	GLY	E	59	54.401	52.216	93.877	1.00	46.55	E
ATOM	7740	N	LYS	E	60	53.185	53.057	92.181	1.00	54.00	E
ATOM	7741	CA	LYS	E	60	54.318	53.146	91.264	1.00	57.19	E
ATOM	7742	CB	LYS	E	60	53.884	53.715	89.910	1.00	57.37	E
ATOM	7743	CG	LYS	E	60	52.787	52.902	89.230	1.00	60.55	E
ATOM	7744	CD	LYS	E	60	52.817	53.027	87.716	1.00	62.15	E
ATOM	7745	CE	LYS	E	60	54.054	52.354	87.136	1.00	73.56	E
ATOM	7746	NZ	LYS	E	60	54.071	52.347	85.637	1.00	79.09	E
ATOM	7747	C	LYS	E	60	55.385	54.033	91.873	1.00	58.12	E
ATOM	7748	O	LYS	E	60	55.223	55.248	91.948	1.00	61.52	E
ATOM	7749	N	LYS	E	61	56.470	53.410	92.314	1.00	54.03	E
ATOM	7750	CA	LYS	E	61	57.571	54.118	92.943	1.00	49.88	E
ATOM	7751	CB	LYS	E	61	57.462	54.013	94.466	1.00	53.55	E
ATOM	7752	CG	LYS	E	61	57.350	55.347	95.189	1.00	60.82	E
ATOM	7753	CD	LYS	E	61	58.333	55.426	96.352	1.00	66.40	E
ATOM	7754	CE	LYS	E	61	58.074	54.343	97.407	1.00	73.51	E
ATOM	7755	NZ	LYS	E	61	59.112	54.322	98.500	1.00	73.88	E
ATOM	7756	C	LYS	E	61	58.869	53.478	92.487	1.00	48.76	E
ATOM	7757	O	LYS	E	61	58.865	52.448	91.813	1.00	47.59	E
ATOM	7758	N	GLU	E	62	59.982	54.092	92.855	1.00	48.58	E
ATOM	7759	CA	GLU	E	62	61.291	53.568	92.493	1.00	48.54	E
ATOM	7760	CB	GLU	E	62	61.758	54.205	91.187	1.00	49.67	E
ATOM	7761	CG	GLU	E	62	62.532	53.266	90.293	1.00	66.30	E
ATOM	7762	CD	GLU	E	62	64.030	53.503	90.345	1.00	74.23	E
ATOM	7763	OE1	GLU	E	62	64.594	53.523	91.464	1.00	81.46	E
ATOM	7764	OE2	GLU	E	62	64.642	53.664	89.262	1.00	72.93	E
ATOM	7765	C	GLU	E	62	62.231	53.911	93.640	1.00	43.78	E
ATOM	7766	O	GLU	E	62	62.229	55.031	94.138	1.00	49.05	E
ATOM	7767	N	ASN	E	63	63.002	52.944	94.103	1.00	39.78	E
ATOM	7768	CA	ASN	E	63	63.921	53.223	95.196	1.00	39.94	E
ATOM	7769	CB	ASN	E	63	63.374	52.781	96.550	1.00	41.74	E
ATOM	7770	CG	ASN	E	63	62.123	53.508	96.939	1.00	46.44	E
ATOM	7771	OD1	ASN	E	63	61.023	53.093	96.594	1.00	52.81	E
ATOM	7772	ND2	ASN	E	63	62.278	54.607	97.660	1.00	48.86	E
ATOM	7773	C	ASN	E	63	65.185	52.475	94.947	1.00	38.50	E
ATOM	7774	O	ASN	E	63	65.254	51.659	94.022	1.00	41.77	E
ATOM	7775	N	THR	E	64	66.175	52.728	95.792	1.00	34.77	E
ATOM	7776	CA	THR	E	64	67.457	52.074	95.635	1.00	35.48	E
ATOM	7777	CB	THR	E	64	68.565	53.087	95.388	1.00	31.59	E
ATOM	7778	OG1	THR	E	64	68.189	53.952	94.310	1.00	43.11	E
ATOM	7779	CG2	THR	E	64	69.853	52.368	95.039	1.00	29.61	E
ATOM	7780	C	THR	E	64	67.903	51.203	96.790	1.00	37.96	E
ATOM	7781	O	THR	E	64	67.898	51.625	97.948	1.00	41.89	E



ATOM	7782	N	LEU	E	65	68.298	49.982	96.456	1.00	38.28	E
ATOM	7783	CA	LEU	E	65	68.805	49.049	97.438	1.00	39.90	E
ATOM	7784	CB	LEU	E	65	68.403	47.627	97.072	1.00	34.15	E
ATOM	7785	CG	LEU	E	65	66.913	47.328	97.194	1.00	33.31	E
ATOM	7786	CD1	LEU	E	65	66.655	45.867	96.904	1.00	32.75	E
ATOM	7787	CD2	LEU	E	65	66.446	47.670	98.590	1.00	39.57	E
ATOM	7788	C	LEU	E	65	70.324	49.186	97.398	1.00	43.55	E
ATOM	7789	O	LEU	E	65	70.895	49.323	96.316	1.00	42.02	E
ATOM	7790	N	ARG	E	66	70.966	49.184	98.568	1.00	45.20	E
ATOM	7791	CA	ARG	E	66	72.419	49.298	98.646	1.00	46.33	E
ATOM	7792	CB	ARG	E	66	72.813	50.546	99.441	1.00	48.13	E
ATOM	7793	CG	ARG	E	66	72.296	51.836	98.836	1.00	53.95	E
ATOM	7794	CD	ARG	E	66	72.547	53.023	99.750	1.00	60.84	E
ATOM	7795	NE	ARG	E	66	71.634	54.132	99.476	1.00	59.54	E
ATOM	7796	CZ	ARG	E	66	71.674	54.880	98.383	1.00	58.20	E
ATOM	7797	NH1	ARG	E	66	72.589	54.640	97.459	1.00	60.32	E
ATOM	7798	NH2	ARG	E	66	70.792	55.859	98.213	1.00	59.58	E
ATOM	7799	C	ARG	E	66	72.977	48.054	99.314	1.00	45.37	E
ATOM	7800	O	ARG	E	66	72.567	47.712	100.428	1.00	47.47	E
ATOM	7801	N	ILE	E	67	73.898	47.378	98.627	1.00	40.37	E
ATOM	7802	CA	ILE	E	67	74.505	46.161	99.149	1.00	41.48	E
ATOM	7803	CB	ILE	E	67	74.751	45.113	98.040	1.00	39.97	E
ATOM	7804	CG2	ILE	E	67	75.517	43.937	98.606	1.00	42.72	E
ATOM	7805	CG1	ILE	E	67	73.427	44.615	97.461	1.00	41.26	E
ATOM	7806	CD1	ILE	E	67	72.791	45.560	96.487	1.00	40.50	E
ATOM	7807	C	ILE	E	67	75.839	46.456	99.825	1.00	44.21	E
ATOM	7808	O	ILE	E	67	76.792	46.931	99.196	1.00	42.82	E
ATOM	7809	N	LEU	E	68	75.911	46.143	101.110	1.00	42.88	E
ATOM	7810	CA	LEU	E	68	77.117	46.398	101.865	1.00	42.67	E
ATOM	7811	CB	LEU	E	68	76.766	47.039	103.196	1.00	43.76	E
ATOM	7812	CG	LEU	E	68	75.778	48.187	103.174	1.00	38.58	E
ATOM	7813	CD1	LEU	E	68	75.549	48.617	104.596	1.00	38.98	E
ATOM	7814	CD2	LEU	E	68	76.315	49.325	102.342	1.00	43.96	E
ATOM	7815	C	LEU	E	68	77.954	45.161	102.126	1.00	44.23	E
ATOM	7816	O	LEU	E	68	77.442	44.098	102.493	1.00	40.01	E
ATOM	7817	N	ASP	E	69	79.260	45.340	101.953	1.00	46.40	E
ATOM	7818	CA	ASP	E	69	80.246	44.301	102.156	1.00	46.31	E
ATOM	7819	CB	ASP	E	69	81.518	44.712	101.430	1.00	45.34	E
ATOM	7820	CG	ASP	E	69	82.667	43.747	101.650	1.00	51.39	E
ATOM	7821	OD1	ASP	E	69	83.730	43.966	101.021	1.00	54.71	E
ATOM	7822	OD2	ASP	E	69	82.521	42.788	102.438	1.00	38.46	E
ATOM	7823	C	ASP	E	69	80.511	44.134	103.643	1.00	49.83	E
ATOM	7824	O	ASP	E	69	81.071	45.012	104.278	1.00	54.01	E
ATOM	7825	N	ALA	E	70	80.097	43.015	104.212	1.00	54.55	E
ATOM	7826	CA	ALA	E	70	80.343	42.780	105.629	1.00	62.04	E
ATOM	7827	CB	ALA	E	70	79.149	42.097	106.274	1.00	59.72	E
ATOM	7828	C	ALA	E	70	81.563	41.887	105.741	1.00	68.47	E
ATOM	7829	O	ALA	E	70	82.299	41.929	106.730	1.00	68.58	E
ATOM	7830	N	THR	E	71	81.767	41.075	104.707	1.00	77.30	E
ATOM	7831	CA	THR	E	71	82.889	40.148	104.664	1.00	83.99	E
ATOM	7832	CB	THR	E	71	82.808	39.197	103.431	1.00	80.64	E
ATOM	7833	OG1	THR	E	71	83.982	38.378	103.385	1.00	80.75	E
ATOM	7834	CG2	THR	E	71	82.685	39.979	102.135	1.00	80.44	E
ATOM	7835	C	THR	E	71	84.212	40.893	104.645	1.00	90.60	E
ATOM	7836	O	THR	E	71	84.633	41.417	103.605	1.00	93.08	E
ATOM	7837	N	ASN	E	72	84.854	40.949	105.809	1.00	94.55	E
ATOM	7838	CA	ASN	E	72	86.136	41.626	105.941	1.00	99.52	E
ATOM	7839	CB	ASN	E	72	86.555	41.670	107.416	1.00	105.13	E



ATOM	7840	CG	ASN	E	72	85.841	42.761	108.198	1.00110.92	E
ATOM	7841	OD1	ASN	E	72	86.064	42.924	109.403	1.00111.97	E
ATOM	7842	ND2	ASN	E	72	84.983	43.521	107.516	1.00112.48	E
ATOM	7843	C	ASN	E	72	87.221	40.932	105.112	1.00100.12	E
ATOM	7844	O	ASN	E	72	88.146	40.326	105.660	1.00101.78	E
ATOM	7845	N	ASN	E	73	87.101	41.022	103.789	1.00 98.06	E
ATOM	7846	CA	ASN	E	73	88.069	40.411	102.883	1.00 94.81	E
ATOM	7847	CB	ASN	E	73	89.339	41.270	102.813	1.00 96.94	E
ATOM	7848	CG	ASN	E	73	89.041	42.761	102.748	1.00 97.49	E
ATOM	7849	OD1	ASN	E	73	88.508	43.345	103.695	1.00 96.53	E
ATOM	7850	ND2	ASN	E	73	89.387	43.382	101.628	1.00 95.84	E
ATOM	7851	C	ASN	E	73	88.437	38.999	103.354	1.00 90.62	E
ATOM	7852	O	ASN	E	73	89.587	38.576	103.231	1.00 90.22	E
ATOM	7853	N	GLN	E	74	87.460	38.280	103.902	1.00 85.30	E
ATOM	7854	CA	GLN	E	74	87.682	36.919	104.395	1.00 80.03	E
ATOM	7855	CB	GLN	E	74	86.814	36.667	105.638	1.00 84.73	E
ATOM	7856	CG	GLN	E	74	87.144	37.616	106.809	1.00 92.54	E
ATOM	7857	CD	GLN	E	74	86.059	37.679	107.889	1.00 94.84	E
ATOM	7858	OE1	GLN	E	74	86.204	38.395	108.887	1.00 92.19	E
ATOM	7859	NE2	GLN	E	74	84.970	36.936	107.690	1.00 92.52	E
ATOM	7860	C	GLN	E	74	87.359	35.898	103.306	1.00 72.13	E
ATOM	7861	O	GLN	E	74	87.261	34.699	103.568	1.00 69.91	E
ATOM	7862	N	LEU	E	75	87.202	36.391	102.080	1.00 63.45	E
ATOM	7863	CA	LEU	E	75	86.881	35.546	100.935	1.00 58.02	E
ATOM	7864	CB	LEU	E	75	85.776	36.189	100.087	1.00 46.47	E
ATOM	7865	CG	LEU	E	75	84.403	36.435	100.705	1.00 42.52	E
ATOM	7866	CD1	LEU	E	75	83.636	37.399	99.843	1.00 34.46	E
ATOM	7867	CD2	LEU	E	75	83.652	35.128	100.867	1.00 38.91	E
ATOM	7868	C	LEU	E	75	88.100	35.347	100.050	1.00 59.56	E
ATOM	7869	O	LEU	E	75	89.051	36.126	100.100	1.00 62.69	E
ATOM	7870	N	PRO	E	76	88.088	34.295	99.222	1.00 58.52	E
ATOM	7871	CD	PRO	E	76	87.078	33.226	99.151	1.00 58.84	E
ATOM	7872	CA	PRO	E	76	89.206	34.019	98.318	1.00 59.64	E
ATOM	7873	CB	PRO	E	76	88.682	32.858	97.484	1.00 58.08	E
ATOM	7874	CG	PRO	E	76	87.834	32.120	98.452	1.00 55.57	E
ATOM	7875	C	PRO	E	76	89.479	35.267	97.466	1.00 62.30	E
ATOM	7876	O	PRO	E	76	88.537	35.919	97.012	1.00 60.80	E
ATOM	7877	N	GLN	E	77	90.752	35.596	97.247	1.00 63.51	E
ATOM	7878	CA	GLN	E	77	91.100	36.780	96.467	1.00 62.98	E
ATOM	7879	CB	GLN	E	77	92.145	37.599	97.217	1.00 61.45	E
ATOM	7880	CG	GLN	E	77	91.627	38.142	98.526	1.00 67.26	E
ATOM	7881	CD	GLN	E	77	90.368	38.967	98.342	1.00 72.26	E
ATOM	7882	OE1	GLN	E	77	89.380	38.786	99.063	1.00 68.32	E
ATOM	7883	NE2	GLN	E	77	90.398	39.886	97.376	1.00 72.34	E
ATOM	7884	C	GLN	E	77	91.578	36.522	95.039	1.00 63.00	E
ATOM	7885	O	GLN	E	77	91.914	37.459	94.316	1.00 63.48	E
ATOM	7886	N	ASP	E	78	91.586	35.260	94.628	1.00 60.29	E
ATOM	7887	CA	ASP	E	78	92.026	34.907	93.289	1.00 58.86	E
ATOM	7888	CB	ASP	E	78	92.912	33.659	93.344	1.00 57.86	E
ATOM	7889	CG	ASP	E	78	92.222	32.477	94.001	1.00 60.35	E
ATOM	7890	OD1	ASP	E	78	92.697	31.338	93.826	1.00 66.03	E
ATOM	7891	OD2	ASP	E	78	91.210	32.675	94.702	1.00 63.50	E
ATOM	7892	C	ASP	E	78	90.860	34.652	92.333	1.00 60.14	E
ATOM	7893	O	ASP	E	78	91.033	34.610	91.113	1.00 61.33	E
ATOM	7894	N	ARG	E	79	89.664	34.496	92.886	1.00 59.24	E
ATOM	7895	CA	ARG	E	79	88.499	34.199	92.070	1.00 53.51	E
ATOM	7896	CB	ARG	E	79	88.288	32.692	92.051	1.00 55.18	E
ATOM	7897	CG	ARG	E	79	87.959	32.121	93.427	1.00 59.32	E



ATOM	7898	CD	ARG	E	79	88.185	30.629	93.479	1.00	60.46	E
ATOM	7899	NE	ARG	E	79	89.613	30.351	93.415	1.00	67.44	E
ATOM	7900	CZ	ARG	E	79	90.140	29.149	93.219	1.00	66.77	E
ATOM	7901	NH1	ARG	E	79	89.355	28.088	93.066	1.00	63.21	E
ATOM	7902	NH2	ARG	E	79	91.458	29.014	93.173	1.00	67.67	E
ATOM	7903	C	ARG	E	79	87.274	34.854	92.652	1.00	47.91	E
ATOM	7904	O	ARG	E	79	87.308	35.349	93.770	1.00	47.61	E
ATOM	7905	N	GLU	E	80	86.186	34.847	91.893	1.00	45.69	E
ATOM	7906	CA	GLU	E	80	84.936	35.425	92.373	1.00	41.83	E
ATOM	7907	CB	GLU	E	80	83.953	35.661	91.232	1.00	36.72	E
ATOM	7908	CG	GLU	E	80	84.422	36.479	90.068	1.00	34.45	E
ATOM	7909	CD	GLU	E	80	83.322	36.623	89.031	1.00	36.06	E
ATOM	7910	OE1	GLU	E	80	82.824	37.753	88.819	1.00	25.44	E
ATOM	7911	OE2	GLU	E	80	82.939	35.590	88.439	1.00	41.97	E
ATOM	7912	C	GLU	E	80	84.289	34.413	93.316	1.00	42.04	E
ATOM	7913	O	GLU	E	80	84.536	33.205	93.221	1.00	40.99	E
ATOM	7914	N	SER	E	81	83.459	34.906	94.224	1.00	38.94	E
ATOM	7915	CA	SER	E	81	82.754	34.024	95.129	1.00	37.54	E
ATOM	7916	CB	SER	E	81	83.036	34.404	96.579	1.00	36.16	E
ATOM	7917	OG	SER	E	81	84.421	34.275	96.866	1.00	46.69	E
ATOM	7918	C	SER	E	81	81.287	34.201	94.787	1.00	37.57	E
ATOM	7919	O	SER	E	81	80.821	35.326	94.602	1.00	39.92	E
ATOM	7920	N	LEU	E	82	80.562	33.094	94.672	1.00	37.80	E
ATOM	7921	CA	LEU	E	82	79.145	33.153	94.330	1.00	37.09	E
ATOM	7922	CB	LEU	E	82	78.725	31.859	93.632	1.00	33.42	E
ATOM	7923	CG	LEU	E	82	77.230	31.579	93.465	1.00	36.62	E
ATOM	7924	CD1	LEU	E	82	76.479	32.766	92.888	1.00	36.62	E
ATOM	7925	CD2	LEU	E	82	77.089	30.387	92.576	1.00	34.16	E
ATOM	7926	C	LEU	E	82	78.234	33.404	95.523	1.00	37.97	E
ATOM	7927	O	LEU	E	82	78.371	32.766	96.572	1.00	36.17	E
ATOM	7928	N	PHE	E	83	77.308	34.345	95.350	1.00	36.70	E
ATOM	7929	CA	PHE	E	83	76.334	34.683	96.383	1.00	36.32	E
ATOM	7930	CB	PHE	E	83	76.724	35.955	97.122	1.00	34.64	E
ATOM	7931	CG	PHE	E	83	77.841	35.765	98.093	1.00	38.99	E
ATOM	7932	CD1	PHE	E	83	79.162	35.718	97.657	1.00	29.61	E
ATOM	7933	CD2	PHE	E	83	77.571	35.603	99.455	1.00	41.22	E
ATOM	7934	CE1	PHE	E	83	80.198	35.508	98.556	1.00	26.15	E
ATOM	7935	CE2	PHE	E	83	78.606	35.392	100.364	1.00	34.51	E
ATOM	7936	CZ	PHE	E	83	79.924	35.346	99.906	1.00	34.28	E
ATOM	7937	C	PHE	E	83	74.974	34.892	95.743	1.00	35.98	E
ATOM	7938	O	PHE	E	83	74.881	35.054	94.535	1.00	35.96	E
ATOM	7939	N	TRP	E	84	73.921	34.891	96.557	1.00	33.53	E
ATOM	7940	CA	TRP	E	84	72.593	35.085	96.034	1.00	27.70	E
ATOM	7941	CB	TRP	E	84	71.794	33.794	96.124	1.00	21.62	E
ATOM	7942	CG	TRP	E	84	72.352	32.728	95.250	1.00	22.88	E
ATOM	7943	CD2	TRP	E	84	72.049	32.491	93.865	1.00	15.47	E
ATOM	7944	CE2	TRP	E	84	72.827	31.390	93.450	1.00	17.90	E
ATOM	7945	CE3	TRP	E	84	71.202	33.101	92.938	1.00	21.85	E
ATOM	7946	CD1	TRP	E	84	73.274	31.795	95.601	1.00	26.81	E
ATOM	7947	NE1	TRP	E	84	73.563	30.981	94.528	1.00	24.54	E
ATOM	7948	CZ2	TRP	E	84	72.782	30.886	92.146	1.00	17.47	E
ATOM	7949	CZ3	TRP	E	84	71.154	32.600	91.644	1.00	9.99	E
ATOM	7950	CH2	TRP	E	84	71.937	31.507	91.262	1.00	17.03	E
ATOM	7951	C	TRP	E	84	71.860	36.206	96.725	1.00	31.06	E
ATOM	7952	O	TRP	E	84	71.710	36.216	97.946	1.00	35.05	E
ATOM	7953	N	MET	E	85	71.404	37.143	95.900	1.00	29.79	E
ATOM	7954	CA	MET	E	85	70.674	38.332	96.300	1.00	26.47	E
ATOM	7955	CB	MET	E	85	71.093	39.468	95.358	1.00	24.99	E



ATOM	7956	CG	MET	E	85	70.302	40.755	95.472	1.00	29.53	E
ATOM	7957	SD	MET	E	85	70.743	41.719	96.891	1.00	40.16	E
ATOM	7958	CE	MET	E	85	69.573	43.093	96.778	1.00	28.55	E
ATOM	7959	C	MET	E	85	69.163	38.042	96.200	1.00	27.49	E
ATOM	7960	O	MET	E	85	68.664	37.582	95.159	1.00	26.09	E
ATOM	7961	N	ASN	E	86	68.442	38.308	97.289	1.00	27.72	E
ATOM	7962	CA	ASN	E	86	66.999	38.064	97.346	1.00	25.63	E
ATOM	7963	CB	ASN	E	86	66.677	36.922	98.341	1.00	22.17	E
ATOM	7964	CG	ASN	E	86	67.237	35.562	97.896	1.00	26.58	E
ATOM	7965	OD1	ASN	E	86	68.420	35.260	98.092	1.00	27.53	E
ATOM	7966	ND2	ASN	E	86	66.385	34.743	97.294	1.00	18.64	E
ATOM	7967	C	ASN	E	86	66.235	39.319	97.741	1.00	23.31	E
ATOM	7968	O	ASN	E	86	66.601	39.994	98.683	1.00	28.66	E
ATOM	7969	N	VAL	E	87	65.174	39.625	97.005	1.00	24.58	E
ATOM	7970	CA	VAL	E	87	64.344	40.798	97.264	1.00	21.63	E
ATOM	7971	CB	VAL	E	87	64.541	41.888	96.177	1.00	21.57	E
ATOM	7972	CG1	VAL	E	87	63.643	43.079	96.444	1.00	11.14	E
ATOM	7973	CG2	VAL	E	87	66.008	42.338	96.144	1.00	13.01	E
ATOM	7974	C	VAL	E	87	62.918	40.283	97.234	1.00	24.89	E
ATOM	7975	O	VAL	E	87	62.406	39.854	96.196	1.00	21.75	E
ATOM	7976	N	LYS	E	88	62.310	40.320	98.414	1.00	27.63	E
ATOM	7977	CA	LYS	E	88	60.961	39.847	98.658	1.00	30.74	E
ATOM	7978	CB	LYS	E	88	60.950	39.114	99.988	1.00	27.69	E
ATOM	7979	CG	LYS	E	88	59.625	38.638	100.467	1.00	30.49	E
ATOM	7980	CD	LYS	E	88	59.869	37.532	101.466	1.00	32.98	E
ATOM	7981	CE	LYS	E	88	58.690	37.316	102.378	1.00	39.50	E
ATOM	7982	NZ	LYS	E	88	59.099	36.365	103.432	1.00	41.12	E
ATOM	7983	C	LYS	E	88	59.961	40.982	98.687	1.00	32.94	E
ATOM	7984	O	LYS	E	88	60.236	42.027	99.270	1.00	36.53	E
ATOM	7985	N	ALA	E	89	58.807	40.778	98.052	1.00	32.23	E
ATOM	7986	CA	ALA	E	89	57.768	41.797	98.031	1.00	34.52	E
ATOM	7987	CB	ALA	E	89	57.294	42.036	96.619	1.00	38.48	E
ATOM	7988	C	ALA	E	89	56.612	41.327	98.892	1.00	36.68	E
ATOM	7989	O	ALA	E	89	55.813	40.489	98.481	1.00	37.19	E
ATOM	7990	N	ILE	E	90	56.525	41.874	100.094	1.00	39.91	E
ATOM	7991	CA	ILE	E	90	55.472	41.498	101.023	1.00	43.86	E
ATOM	7992	CB	ILE	E	90	55.944	41.669	102.481	1.00	41.73	E
ATOM	7993	CG2	ILE	E	90	54.807	41.348	103.435	1.00	37.50	E
ATOM	7994	CG1	ILE	E	90	57.153	40.770	102.749	1.00	41.42	E
ATOM	7995	CD1	ILE	E	90	57.772	40.959	104.123	1.00	36.06	E
ATOM	7996	C	ILE	E	90	54.195	42.318	100.839	1.00	49.62	E
ATOM	7997	O	ILE	E	90	54.196	43.552	100.973	1.00	53.43	E
ATOM	7998	N	PRO	E	91	53.080	41.646	100.528	1.00	50.88	E
ATOM	7999	CD	PRO	E	91	52.876	40.228	100.200	1.00	47.40	E
ATOM	8000	CA	PRO	E	91	51.846	42.405	100.356	1.00	52.77	E
ATOM	8001	CB	PRO	E	91	50.930	41.410	99.667	1.00	43.99	E
ATOM	8002	CG	PRO	E	91	51.373	40.127	100.231	1.00	47.25	E
ATOM	8003	C	PRO	E	91	51.332	42.850	101.722	1.00	58.30	E
ATOM	8004	O	PRO	E	91	52.105	43.050	102.651	1.00	59.29	E
ATOM	8005	N	SER	E	92	50.026	43.012	101.842	1.00	66.75	E
ATOM	8006	CA	SER	E	92	49.423	43.443	103.092	1.00	70.53	E
ATOM	8007	CB	SER	E	92	49.103	44.932	102.993	1.00	71.10	E
ATOM	8008	OG	SER	E	92	48.760	45.264	101.652	1.00	72.77	E
ATOM	8009	C	SER	E	92	48.163	42.625	103.309	1.00	74.39	E
ATOM	8010	O	SER	E	92	47.531	42.217	102.342	1.00	78.28	E
ATOM	8011	N	MET	E	93	47.798	42.378	104.563	1.00	79.36	E
ATOM	8012	CA	MET	E	93	46.609	41.577	104.869	1.00	84.73	E
ATOM	8013	CB	MET	E	93	46.667	41.073	106.323	1.00	90.59	E



ATOM	8014	CG	MET	E	93	45.718	39.902	106.647	1.00	99.54	E
ATOM	8015	SD	MET	E	93	44.009	40.307	107.183	1.00	107.95	E
ATOM	8016	CE	MET	E	93	43.997	39.613	108.839	1.00	102.16	E
ATOM	8017	C	MET	E	93	45.304	42.339	104.646	1.00	85.19	E
ATOM	8018	O	MET	E	93	45.100	43.411	105.218	1.00	83.73	E
ATOM	8019	N	ASP	E	94	44.431	41.786	103.802	1.00	87.08	E
ATOM	8020	CA	ASP	E	94	43.135	42.404	103.536	1.00	87.83	E
ATOM	8021	CB	ASP	E	94	42.395	41.739	102.363	1.00	88.98	E
ATOM	8022	CG	ASP	E	94	43.155	41.815	101.051	1.00	93.19	E
ATOM	8023	OD1	ASP	E	94	42.492	41.873	99.988	1.00	89.53	E
ATOM	8024	OD2	ASP	E	94	44.405	41.796	101.076	1.00	95.08	E
ATOM	8025	C	ASP	E	94	42.290	42.190	104.776	1.00	87.87	E
ATOM	8026	O	ASP	E	94	42.071	41.051	105.189	1.00	86.91	E
ATOM	8027	N	LYS	E	95	41.828	43.273	105.384	1.00	89.56	E
ATOM	8028	CA	LYS	E	95	40.972	43.148	106.552	1.00	89.71	E
ATOM	8029	CB	LYS	E	95	40.931	44.464	107.327	1.00	89.46	E
ATOM	8030	CG	LYS	E	95	42.221	44.798	108.058	1.00	87.67	E
ATOM	8031	CD	LYS	E	95	43.332	45.235	107.129	1.00	90.85	E
ATOM	8032	CE	LYS	E	95	43.085	46.633	106.578	1.00	90.41	E
ATOM	8033	NZ	LYS	E	95	44.257	47.140	105.806	1.00	90.02	E
ATOM	8034	C	LYS	E	95	39.601	42.825	105.973	1.00	90.47	E
ATOM	8035	O	LYS	E	95	38.619	42.681	106.692	1.00	90.02	E
ATOM	8036	N	SER	E	96	39.574	42.704	104.648	1.00	92.81	E
ATOM	8037	CA	SER	E	96	38.369	42.409	103.878	1.00	93.23	E
ATOM	8038	CB	SER	E	96	38.459	43.086	102.501	1.00	92.72	E
ATOM	8039	OG	SER	E	96	39.652	42.728	101.817	1.00	90.65	E
ATOM	8040	C	SER	E	96	38.074	40.916	103.686	1.00	93.41	E
ATOM	8041	O	SER	E	96	36.907	40.513	103.646	1.00	94.89	E
ATOM	8042	N	LYS	E	97	39.116	40.099	103.551	1.00	91.56	E
ATOM	8043	CA	LYS	E	97	38.923	38.665	103.355	1.00	90.60	E
ATOM	8044	CB	LYS	E	97	39.802	38.162	102.208	1.00	92.72	E
ATOM	8045	CG	LYS	E	97	39.782	39.029	100.953	1.00	97.27	E
ATOM	8046	CD	LYS	E	97	38.398	39.132	100.337	1.00	102.20	E
ATOM	8047	CE	LYS	E	97	38.419	40.032	99.108	1.00	105.13	E
ATOM	8048	NZ	LYS	E	97	37.056	40.261	98.549	1.00	106.19	E
ATOM	8049	C	LYS	E	97	39.273	37.917	104.636	1.00	88.83	E
ATOM	8050	O	LYS	E	97	39.449	36.700	104.635	1.00	88.67	E
ATOM	8051	N	LEU	E	98	39.353	38.670	105.726	1.00	87.92	E
ATOM	8052	CA	LEU	E	98	39.697	38.159	107.049	1.00	88.15	E
ATOM	8053	CB	LEU	E	98	39.498	39.290	108.069	1.00	91.70	E
ATOM	8054	CG	LEU	E	98	39.764	39.077	109.563	1.00	94.58	E
ATOM	8055	CD1	LEU	E	98	38.557	38.427	110.209	1.00	93.87	E
ATOM	8056	CD2	LEU	E	98	41.027	38.243	109.756	1.00	95.95	E
ATOM	8057	C	LEU	E	98	38.989	36.876	107.522	1.00	86.75	E
ATOM	8058	O	LEU	E	98	39.641	35.985	108.076	1.00	86.39	E
ATOM	8059	N	THR	E	99	37.673	36.779	107.319	1.00	84.26	E
ATOM	8060	CA	THR	E	99	36.917	35.594	107.746	1.00	81.01	E
ATOM	8061	CB	THR	E	99	35.512	35.959	108.291	1.00	84.06	E
ATOM	8062	OG1	THR	E	99	34.695	36.447	107.216	1.00	85.84	E
ATOM	8063	CG2	THR	E	99	35.609	37.025	109.385	1.00	79.28	E
ATOM	8064	C	THR	E	99	36.726	34.652	106.569	1.00	78.00	E
ATOM	8065	O	THR	E	99	35.733	33.930	106.477	1.00	75.16	E
ATOM	8066	N	GLU	E	100	37.690	34.678	105.661	1.00	77.82	E
ATOM	8067	CA	GLU	E	100	37.647	33.839	104.478	1.00	76.57	E
ATOM	8068	CB	GLU	E	100	37.577	34.709	103.222	1.00	79.22	E
ATOM	8069	CG	GLU	E	100	36.223	35.351	102.979	1.00	85.62	E
ATOM	8070	CD	GLU	E	100	36.250	36.355	101.841	1.00	85.86	E
ATOM	8071	OE1	GLU	E	100	36.732	36.004	100.743	1.00	88.66	E



ATOM	8072	OE2	GLU	E	100	35.783	37.496	102.046	1.00	87.70	E
ATOM	8073	C	GLU	E	100	38.864	32.942	104.380	1.00	72.88	E
ATOM	8074	O	GLU	E	100	39.874	33.168	105.039	1.00	72.40	E
ATOM	8075	N	ASN	E	101	38.750	31.912	103.555	1.00	70.72	E
ATOM	8076	CA	ASN	E	101	39.853	31.000	103.319	1.00	68.45	E
ATOM	8077	CB	ASN	E	101	39.324	29.650	102.860	1.00	69.36	E
ATOM	8078	CG	ASN	E	101	39.153	28.687	104.008	1.00	72.47	E
ATOM	8079	OD1	ASN	E	101	38.993	29.101	105.162	1.00	70.21	E
ATOM	8080	ND2	ASN	E	101	39.186	27.393	103.705	1.00	71.50	E
ATOM	8081	C	ASN	E	101	40.654	31.661	102.221	1.00	65.35	E
ATOM	8082	O	ASN	E	101	40.173	31.799	101.093	1.00	64.51	E
ATOM	8083	N	THR	E	102	41.871	32.078	102.551	1.00	61.53	E
ATOM	8084	CA	THR	E	102	42.706	32.783	101.585	1.00	58.27	E
ATOM	8085	CB	THR	E	102	42.834	34.260	101.977	1.00	59.49	E
ATOM	8086	OG1	THR	E	102	43.418	34.351	103.282	1.00	65.49	E
ATOM	8087	CG2	THR	E	102	41.471	34.923	102.014	1.00	63.21	E
ATOM	8088	C	THR	E	102	44.112	32.250	101.376	1.00	53.56	E
ATOM	8089	O	THR	E	102	44.652	31.497	102.193	1.00	46.83	E
ATOM	8090	N	LEU	E	103	44.686	32.646	100.245	1.00	53.52	E
ATOM	8091	CA	LEU	E	103	46.060	32.287	99.894	1.00	52.79	E
ATOM	8092	CB	LEU	E	103	46.137	31.252	98.766	1.00	47.71	E
ATOM	8093	CG	LEU	E	103	47.580	31.081	98.263	1.00	45.50	E
ATOM	8094	CD1	LEU	E	103	48.432	30.438	99.373	1.00	48.21	E
ATOM	8095	CD2	LEU	E	103	47.611	30.240	97.010	1.00	42.09	E
ATOM	8096	C	LEU	E	103	46.771	33.531	99.412	1.00	50.34	E
ATOM	8097	O	LEU	E	103	46.315	34.195	98.484	1.00	49.12	E
ATOM	8098	N	GLN	E	104	47.882	33.862	100.046	1.00	51.12	E
ATOM	8099	CA	GLN	E	104	48.629	35.017	99.595	1.00	49.91	E
ATOM	8100	CB	GLN	E	104	48.733	36.066	100.697	1.00	52.16	E
ATOM	8101	CG	GLN	E	104	47.932	37.316	100.364	1.00	52.81	E
ATOM	8102	CD	GLN	E	104	48.101	38.420	101.385	1.00	52.39	E
ATOM	8103	OE1	GLN	E	104	47.562	39.513	101.220	1.00	50.17	E
ATOM	8104	NE2	GLN	E	104	48.852	38.142	102.447	1.00	49.23	E
ATOM	8105	C	GLN	E	104	50.010	34.602	99.131	1.00	45.45	E
ATOM	8106	O	GLN	E	104	50.643	33.724	99.721	1.00	42.43	E
ATOM	8107	N	LEU	E	105	50.461	35.218	98.050	1.00	40.23	E
ATOM	8108	CA	LEU	E	105	51.777	34.919	97.539	1.00	38.09	E
ATOM	8109	CB	LEU	E	105	51.726	34.674	96.036	1.00	37.00	E
ATOM	8110	CG	LEU	E	105	50.889	33.484	95.566	1.00	36.98	E
ATOM	8111	CD1	LEU	E	105	51.067	33.328	94.077	1.00	39.35	E
ATOM	8112	CD2	LEU	E	105	51.321	32.210	96.266	1.00	43.30	E
ATOM	8113	C	LEU	E	105	52.683	36.102	97.826	1.00	35.91	E
ATOM	8114	O	LEU	E	105	52.223	37.221	97.961	1.00	39.57	E
ATOM	8115	N	ALA	E	106	53.970	35.825	97.956	1.00	34.03	E
ATOM	8116	CA	ALA	E	106	54.989	36.836	98.187	1.00	28.24	E
ATOM	8117	CB	ALA	E	106	55.600	36.680	99.576	1.00	24.61	E
ATOM	8118	C	ALA	E	106	56.036	36.559	97.116	1.00	29.64	E
ATOM	8119	O	ALA	E	106	56.761	35.551	97.161	1.00	31.55	E
ATOM	8120	N	ILE	E	107	56.100	37.435	96.129	1.00	29.04	E
ATOM	8121	CA	ILE	E	107	57.055	37.250	95.056	1.00	25.15	E
ATOM	8122	CB	ILE	E	107	56.688	38.085	93.838	1.00	24.58	E
ATOM	8123	CG2	ILE	E	107	57.473	37.585	92.622	1.00	26.45	E
ATOM	8124	CG1	ILE	E	107	55.190	37.966	93.559	1.00	22.85	E
ATOM	8125	CD1	ILE	E	107	54.765	36.580	93.092	1.00	23.65	E
ATOM	8126	C	ILE	E	107	58.425	37.680	95.528	1.00	27.52	E
ATOM	8127	O	ILE	E	107	58.569	38.671	96.254	1.00	29.67	E
ATOM	8128	N	ILE	E	108	59.433	36.933	95.106	1.00	28.37	E
ATOM	8129	CA	ILE	E	108	60.808	37.239	95.465	1.00	30.65	E



ATOM	8130	CB	ILE	E	108	61.363	36.201	96.470	1.00	31.17	E
ATOM	8131	CG2	ILE	E	108	62.770	36.590	96.903	1.00	20.29	E
ATOM	8132	CG1	ILE	E	108	60.403	36.068	97.661	1.00	28.26	E
ATOM	8133	CD1	ILE	E	108	60.653	34.821	98.509	1.00	19.06	E
ATOM	8134	C	ILE	E	108	61.660	37.171	94.206	1.00	29.17	E
ATOM	8135	O	ILE	E	108	61.420	36.331	93.337	1.00	27.52	E
ATOM	8136	N	SER	E	109	62.644	38.054	94.097	1.00	29.12	E
ATOM	8137	CA	SER	E	109	63.542	38.007	92.945	1.00	28.65	E
ATOM	8138	CB	SER	E	109	63.652	39.378	92.282	1.00	25.60	E
ATOM	8139	OG	SER	E	109	62.372	39.852	91.889	1.00	29.24	E
ATOM	8140	C	SER	E	109	64.870	37.593	93.566	1.00	28.87	E
ATOM	8141	O	SER	E	109	65.300	38.181	94.563	1.00	30.52	E
ATOM	8142	N	ARG	E	110	65.477	36.545	93.021	1.00	24.79	E
ATOM	8143	CA	ARG	E	110	66.746	36.039	93.521	1.00	27.37	E
ATOM	8144	CB	ARG	E	110	66.601	34.599	94.047	1.00	25.59	E
ATOM	8145	CG	ARG	E	110	67.849	33.730	93.788	1.00	30.47	E
ATOM	8146	CD	ARG	E	110	67.781	32.339	94.401	1.00	23.46	E
ATOM	8147	NE	ARG	E	110	67.741	32.440	95.852	1.00	29.94	E
ATOM	8148	CZ	ARG	E	110	68.591	31.850	96.686	1.00	29.72	E
ATOM	8149	NH1	ARG	E	110	69.578	31.085	96.237	1.00	16.98	E
ATOM	8150	NH2	ARG	E	110	68.458	32.061	97.984	1.00	24.90	E
ATOM	8151	C	ARG	E	110	67.747	36.060	92.375	1.00	33.03	E
ATOM	8152	O	ARG	E	110	67.583	35.347	91.373	1.00	31.91	E
ATOM	8153	N	ILE	E	111	68.791	36.871	92.533	1.00	34.02	E
ATOM	8154	CA	ILE	E	111	69.807	36.984	91.505	1.00	31.29	E
ATOM	8155	CB	ILE	E	111	69.737	38.356	90.859	1.00	32.17	E
ATOM	8156	CG2	ILE	E	111	68.370	38.535	90.181	1.00	32.88	E
ATOM	8157	CG1	ILE	E	111	69.967	39.428	91.920	1.00	32.03	E
ATOM	8158	CD1	ILE	E	111	70.100	40.828	91.349	1.00	27.85	E
ATOM	8159	C	ILE	E	111	71.217	36.746	92.018	1.00	27.76	E
ATOM	8160	O	ILE	E	111	71.495	36.905	93.201	1.00	29.85	E
ATOM	8161	N	LYS	E	112	72.109	36.363	91.118	1.00	26.03	E
ATOM	8162	CA	LYS	E	112	73.487	36.115	91.494	1.00	28.03	E
ATOM	8163	CB	LYS	E	112	74.249	35.460	90.353	1.00	26.10	E
ATOM	8164	CG	LYS	E	112	73.547	34.310	89.684	1.00	28.45	E
ATOM	8165	CD	LYS	E	112	74.371	33.862	88.492	1.00	35.18	E
ATOM	8166	CE	LYS	E	112	73.690	32.776	87.701	1.00	44.85	E
ATOM	8167	NZ	LYS	E	112	74.524	32.371	86.528	1.00	45.06	E
ATOM	8168	C	LYS	E	112	74.198	37.413	91.855	1.00	27.69	E
ATOM	8169	O	LYS	E	112	73.945	38.468	91.292	1.00	32.27	E
ATOM	8170	N	LEU	E	113	75.086	37.321	92.819	1.00	26.20	E
ATOM	8171	CA	LEU	E	113	75.868	38.452	93.244	1.00	30.07	E
ATOM	8172	CB	LEU	E	113	75.437	38.903	94.633	1.00	26.50	E
ATOM	8173	CG	LEU	E	113	76.385	39.835	95.386	1.00	28.06	E
ATOM	8174	CD1	LEU	E	113	76.998	40.835	94.438	1.00	40.23	E
ATOM	8175	CD2	LEU	E	113	75.614	40.573	96.457	1.00	34.89	E
ATOM	8176	C	LEU	E	113	77.290	37.912	93.277	1.00	35.19	E
ATOM	8177	O	LEU	E	113	77.567	36.962	94.011	1.00	43.89	E
ATOM	8178	N	TYR	E	114	78.180	38.461	92.458	1.00	30.39	E
ATOM	8179	CA	TYR	E	114	79.548	37.973	92.492	1.00	34.53	E
ATOM	8180	CB	TYR	E	114	80.130	37.763	91.091	1.00	31.04	E
ATOM	8181	CG	TYR	E	114	79.407	36.767	90.235	1.00	29.75	E
ATOM	8182	CD1	TYR	E	114	78.646	37.187	89.145	1.00	27.37	E
ATOM	8183	CE1	TYR	E	114	77.976	36.281	88.353	1.00	23.53	E
ATOM	8184	CD2	TYR	E	114	79.482	35.405	90.504	1.00	28.01	E
ATOM	8185	CE2	TYR	E	114	78.814	34.480	89.706	1.00	25.24	E
ATOM	8186	CZ	TYR	E	114	78.063	34.931	88.636	1.00	27.63	E
ATOM	8187	OH	TYR	E	114	77.384	34.042	87.839	1.00	33.91	E



ATOM	8188	C	TYR	E	114	80.448	38.949	93.221	1.00	38.12	E
ATOM	8189	O	TYR	E	114	80.372	40.166	93.021	1.00	38.72	E
ATOM	8190	N	TYR	E	115	81.289	38.403	94.083	1.00	40.23	E
ATOM	8191	CA	TYR	E	115	82.269	39.194	94.802	1.00	41.88	E
ATOM	8192	CB	TYR	E	115	82.583	38.541	96.143	1.00	40.46	E
ATOM	8193	CG	TYR	E	115	83.665	39.239	96.912	1.00	45.20	E
ATOM	8194	CD1	TYR	E	115	83.418	40.468	97.531	1.00	47.84	E
ATOM	8195	CE1	TYR	E	115	84.402	41.123	98.248	1.00	49.89	E
ATOM	8196	CD2	TYR	E	115	84.941	38.678	97.030	1.00	43.74	E
ATOM	8197	CE2	TYR	E	115	85.940	39.326	97.747	1.00	46.84	E
ATOM	8198	CZ	TYR	E	115	85.664	40.552	98.355	1.00	51.90	E
ATOM	8199	OH	TYR	E	115	86.644	41.217	99.060	1.00	57.44	E
ATOM	8200	C	TYR	E	115	83.458	39.035	93.859	1.00	43.51	E
ATOM	8201	O	TYR	E	115	83.998	37.939	93.717	1.00	47.45	E
ATOM	8202	N	ARG	E	116	83.847	40.105	93.182	1.00	46.54	E
ATOM	8203	CA	ARG	E	116	84.960	40.022	92.244	1.00	48.67	E
ATOM	8204	CB	ARG	E	116	84.577	40.676	90.916	1.00	50.62	E
ATOM	8205	CG	ARG	E	116	85.669	40.636	89.855	1.00	55.10	E
ATOM	8206	CD	ARG	E	116	85.126	41.074	88.506	1.00	48.73	E
ATOM	8207	NE	ARG	E	116	84.197	40.087	87.974	1.00	49.25	E
ATOM	8208	CZ	ARG	E	116	83.268	40.353	87.063	1.00	47.27	E
ATOM	8209	NH1	ARG	E	116	83.150	41.583	86.590	1.00	45.04	E
ATOM	8210	NH2	ARG	E	116	82.462	39.390	86.623	1.00	44.03	E
ATOM	8211	C	ARG	E	116	86.217	40.667	92.783	1.00	50.92	E
ATOM	8212	O	ARG	E	116	86.341	41.885	92.792	1.00	51.75	E
ATOM	8213	N	PRO	E	117	87.168	39.851	93.252	1.00	56.58	E
ATOM	8214	CD	PRO	E	117	87.192	38.379	93.241	1.00	58.31	E
ATOM	8215	CA	PRO	E	117	88.422	40.387	93.790	1.00	62.30	E
ATOM	8216	CB	PRO	E	117	89.293	39.141	93.956	1.00	59.71	E
ATOM	8217	CG	PRO	E	117	88.303	38.073	94.223	1.00	59.53	E
ATOM	8218	C	PRO	E	117	89.007	41.346	92.771	1.00	65.34	E
ATOM	8219	O	PRO	E	117	89.511	40.920	91.742	1.00	67.65	E
ATOM	8220	N	ALA	E	118	88.916	42.637	93.040	1.00	71.43	E
ATOM	8221	CA	ALA	E	118	89.451	43.623	92.115	1.00	77.39	E
ATOM	8222	CB	ALA	E	118	88.963	45.025	92.504	1.00	82.03	E
ATOM	8223	C	ALA	E	118	90.977	43.555	92.154	1.00	79.41	E
ATOM	8224	O	ALA	E	118	91.606	44.229	92.974	1.00	79.28	E
ATOM	8225	N	LYS	E	119	91.559	42.737	91.270	1.00	80.34	E
ATOM	8226	CA	LYS	E	119	93.011	42.559	91.194	1.00	79.09	E
ATOM	8227	CB	LYS	E	119	93.580	42.328	92.596	1.00	79.93	E
ATOM	8228	CG	LYS	E	119	95.067	42.627	92.749	1.00	82.41	E
ATOM	8229	CD	LYS	E	119	95.339	44.119	92.887	1.00	81.91	E
ATOM	8230	CE	LYS	E	119	96.767	44.373	93.376	1.00	84.83	E
ATOM	8231	NZ	LYS	E	119	97.051	45.806	93.688	1.00	86.64	E
ATOM	8232	C	LYS	E	119	93.362	41.357	90.311	1.00	79.42	E
ATOM	8233	O	LYS	E	119	94.475	40.829	90.375	1.00	80.69	E
ATOM	8234	N	LEU	E	120	92.418	40.929	89.482	1.00	78.31	E
ATOM	8235	CA	LEU	E	120	92.639	39.773	88.617	1.00	76.92	E
ATOM	8236	CB	LEU	E	120	91.326	39.011	88.435	1.00	78.87	E
ATOM	8237	CG	LEU	E	120	90.520	38.821	89.725	1.00	78.12	E
ATOM	8238	CD1	LEU	E	120	89.227	38.091	89.422	1.00	77.81	E
ATOM	8239	CD2	LEU	E	120	91.345	38.056	90.745	1.00	77.20	E
ATOM	8240	C	LEU	E	120	93.195	40.176	87.258	1.00	75.89	E
ATOM	8241	O	LEU	E	120	92.919	41.271	86.759	1.00	75.25	E
ATOM	8242	N	ALA	E	121	93.974	39.278	86.660	1.00	74.37	E
ATOM	8243	CA	ALA	E	121	94.595	39.537	85.363	1.00	71.38	E
ATOM	8244	CB	ALA	E	121	95.741	38.557	85.135	1.00	71.37	E
ATOM	8245	C	ALA	E	121	93.609	39.451	84.210	1.00	67.34	E



ATOM	8246	O	ALA	E	121	93.230	40.456	83.621	1.00	65.61	E
ATOM	8247	N	LEU	E	122	93.201	38.235	83.891	1.00	66.30	E
ATOM	8248	CA	LEU	E	122	92.273	38.009	82.802	1.00	67.41	E
ATOM	8249	CB	LEU	E	122	91.902	36.529	82.756	1.00	67.53	E
ATOM	8250	CG	LEU	E	122	90.736	36.126	81.856	1.00	71.32	E
ATOM	8251	CD1	LEU	E	122	90.764	36.927	80.566	1.00	69.46	E
ATOM	8252	CD2	LEU	E	122	90.817	34.628	81.584	1.00	72.73	E
ATOM	8253	C	LEU	E	122	91.017	38.858	82.907	1.00	67.54	E
ATOM	8254	O	LEU	E	122	90.185	38.629	83.768	1.00	70.87	E
ATOM	8255	N	PRO	E	123	90.860	39.848	82.018	1.00	68.07	E
ATOM	8256	CD	PRO	E	123	91.771	40.218	80.920	1.00	69.16	E
ATOM	8257	CA	PRO	E	123	89.680	40.721	82.033	1.00	68.69	E
ATOM	8258	CB	PRO	E	123	90.065	41.822	81.048	1.00	69.48	E
ATOM	8259	CG	PRO	E	123	90.884	41.084	80.039	1.00	69.70	E
ATOM	8260	C	PRO	E	123	88.397	39.973	81.623	1.00	67.34	E
ATOM	8261	O	PRO	E	123	88.363	39.288	80.599	1.00	67.21	E
ATOM	8262	N	PRO	E	124	87.325	40.117	82.416	1.00	64.53	E
ATOM	8263	CD	PRO	E	124	87.209	41.151	83.453	1.00	63.28	E
ATOM	8264	CA	PRO	E	124	86.026	39.476	82.191	1.00	63.28	E
ATOM	8265	CB	PRO	E	124	85.050	40.370	82.966	1.00	62.47	E
ATOM	8266	CG	PRO	E	124	85.817	41.631	83.226	1.00	65.30	E
ATOM	8267	C	PRO	E	124	85.604	39.259	80.742	1.00	63.28	E
ATOM	8268	O	PRO	E	124	85.061	38.208	80.395	1.00	60.22	E
ATOM	8269	N	ASP	E	125	85.842	40.250	79.899	1.00	66.27	E
ATOM	8270	CA	ASP	E	125	85.491	40.146	78.485	1.00	71.14	E
ATOM	8271	CB	ASP	E	125	85.960	41.398	77.772	1.00	77.36	E
ATOM	8272	CG	ASP	E	125	87.425	41.673	78.028	1.00	84.23	E
ATOM	8273	OD1	ASP	E	125	88.286	40.920	77.517	1.00	86.56	E
ATOM	8274	OD2	ASP	E	125	87.720	42.635	78.764	1.00	90.78	E
ATOM	8275	C	ASP	E	125	86.184	38.947	77.843	1.00	72.05	E
ATOM	8276	O	ASP	E	125	85.633	38.271	76.972	1.00	71.71	E
ATOM	8277	N	GLN	E	126	87.406	38.704	78.294	1.00	72.31	E
ATOM	8278	CA	GLN	E	126	88.257	37.644	77.780	1.00	74.02	E
ATOM	8279	CB	GLN	E	126	89.702	38.172	77.843	1.00	79.69	E
ATOM	8280	CG	GLN	E	126	90.810	37.336	77.190	1.00	86.00	E
ATOM	8281	CD	GLN	E	126	92.171	38.029	77.289	1.00	87.14	E
ATOM	8282	OE1	GLN	E	126	93.222	37.417	77.062	1.00	87.09	E
ATOM	8283	NE2	GLN	E	126	92.150	39.318	77.624	1.00	86.89	E
ATOM	8284	C	GLN	E	126	88.111	36.305	78.527	1.00	72.95	E
ATOM	8285	O	GLN	E	126	89.083	35.560	78.665	1.00	74.41	E
ATOM	8286	N	ALA	E	127	86.903	35.984	78.991	1.00	70.16	E
ATOM	8287	CA	ALA	E	127	86.692	34.742	79.739	1.00	65.81	E
ATOM	8288	CB	ALA	E	127	85.986	35.044	81.050	1.00	59.82	E
ATOM	8289	C	ALA	E	127	85.956	33.622	78.997	1.00	64.60	E
ATOM	8290	O	ALA	E	127	86.378	32.469	79.040	1.00	63.08	E
ATOM	8291	N	ALA	E	128	84.866	33.948	78.315	1.00	64.06	E
ATOM	8292	CA	ALA	E	128	84.109	32.932	77.590	1.00	66.61	E
ATOM	8293	CB	ALA	E	128	82.996	33.589	76.788	1.00	62.84	E
ATOM	8294	C	ALA	E	128	84.992	32.080	76.665	1.00	70.89	E
ATOM	8295	O	ALA	E	128	84.826	30.859	76.587	1.00	70.48	E
ATOM	8296	N	GLU	E	129	85.930	32.726	75.976	1.00	74.32	E
ATOM	8297	CA	GLU	E	129	86.837	32.047	75.050	1.00	75.77	E
ATOM	8298	CB	GLU	E	129	87.841	33.033	74.472	1.00	81.67	E
ATOM	8299	CG	GLU	E	129	87.390	34.477	74.491	1.00	97.61	E
ATOM	8300	CD	GLU	E	129	88.565	35.447	74.471	1.00	103.11	E
ATOM	8301	OE1	GLU	E	129	88.331	36.664	74.278	1.00	107.16	E
ATOM	8302	OE2	GLU	E	129	89.719	34.990	74.662	1.00	104.91	E
ATOM	8303	C	GLU	E	129	87.631	30.942	75.730	1.00	75.65	E



ATOM	8304	O	GLU	E	129	87.826	29.863	75.163	1.00	76.89	E
ATOM	8305	N	LYS	E	130	88.108	31.231	76.938	1.00	71.46	E
ATOM	8306	CA	LYS	E	130	88.911	30.288	77.703	1.00	68.34	E
ATOM	8307	CB	LYS	E	130	89.385	30.939	79.002	1.00	72.68	E
ATOM	8308	CG	LYS	E	130	90.110	32.270	78.817	1.00	76.69	E
ATOM	8309	CD	LYS	E	130	91.477	32.083	78.179	1.00	78.95	E
ATOM	8310	CE	LYS	E	130	92.154	33.415	77.900	1.00	80.02	E
ATOM	8311	NZ	LYS	E	130	93.512	33.220	77.309	1.00	80.28	E
ATOM	8312	C	LYS	E	130	88.170	29.007	78.038	1.00	66.39	E
ATOM	8313	O	LYS	E	130	88.742	28.104	78.641	1.00	66.28	E
ATOM	8314	N	LEU	E	131	86.904	28.926	77.642	1.00	64.93	E
ATOM	8315	CA	LEU	E	131	86.092	27.751	77.928	1.00	66.19	E
ATOM	8316	CB	LEU	E	131	84.604	28.070	77.781	1.00	63.41	E
ATOM	8317	CG	LEU	E	131	83.700	26.931	78.275	1.00	59.42	E
ATOM	8318	CD1	LEU	E	131	83.805	26.830	79.799	1.00	54.50	E
ATOM	8319	CD2	LEU	E	131	82.267	27.178	77.850	1.00	56.06	E
ATOM	8320	C	LEU	E	131	86.398	26.557	77.049	1.00	69.57	E
ATOM	8321	O	LEU	E	131	86.045	26.544	75.873	1.00	74.49	E
ATOM	8322	N	ARG	E	132	87.031	25.544	77.624	1.00	72.41	E
ATOM	8323	CA	ARG	E	132	87.357	24.336	76.877	1.00	78.60	E
ATOM	8324	CB	ARG	E	132	88.748	23.836	77.273	1.00	83.64	E
ATOM	8325	CG	ARG	E	132	89.846	24.882	77.138	1.00	89.83	E
ATOM	8326	CD	ARG	E	132	91.098	24.466	77.907	1.00	96.13	E
ATOM	8327	NE	ARG	E	132	91.968	25.607	78.196	1.00	100.26	E
ATOM	8328	CZ	ARG	E	132	93.006	25.569	79.029	1.00	101.37	E
ATOM	8329	NH1	ARG	E	132	93.316	24.443	79.664	1.00	100.07	E
ATOM	8330	NH2	ARG	E	132	93.727	26.664	79.239	1.00	102.77	E
ATOM	8331	C	ARG	E	132	86.305	23.268	77.180	1.00	79.65	E
ATOM	8332	O	ARG	E	132	85.317	23.539	77.863	1.00	78.67	E
ATOM	8333	N	PHE	E	133	86.511	22.055	76.678	1.00	81.70	E
ATOM	8334	CA	PHE	E	133	85.555	20.979	76.912	1.00	86.89	E
ATOM	8335	CB	PHE	E	133	84.550	20.906	75.759	1.00	86.42	E
ATOM	8336	CG	PHE	E	133	83.637	22.090	75.674	1.00	86.29	E
ATOM	8337	CD1	PHE	E	133	84.110	23.320	75.237	1.00	86.42	E
ATOM	8338	CD2	PHE	E	133	82.304	21.981	76.057	1.00	88.13	E
ATOM	8339	CE1	PHE	E	133	83.272	24.427	75.182	1.00	88.07	E
ATOM	8340	CE2	PHE	E	133	81.453	23.078	76.008	1.00	88.03	E
ATOM	8341	CZ	PHE	E	133	81.937	24.307	75.570	1.00	88.68	E
ATOM	8342	C	PHE	E	133	86.168	19.595	77.126	1.00	91.17	E
ATOM	8343	O	PHE	E	133	87.358	19.452	77.412	1.00	93.88	E
ATOM	8344	N	ARG	E	134	85.321	18.581	76.985	1.00	92.71	E
ATOM	8345	CA	ARG	E	134	85.689	17.178	77.148	1.00	95.08	E
ATOM	8346	CB	ARG	E	134	86.147	16.903	78.575	1.00	91.89	E
ATOM	8347	CG	ARG	E	134	86.322	15.433	78.889	1.00	91.75	E
ATOM	8348	CD	ARG	E	134	86.312	15.220	80.391	1.00	95.21	E
ATOM	8349	NE	ARG	E	134	87.383	15.960	81.052	1.00	98.21	E
ATOM	8350	CZ	ARG	E	134	87.388	16.268	82.345	1.00	99.25	E
ATOM	8351	NH1	ARG	E	134	86.372	15.903	83.119	1.00	98.61	E
ATOM	8352	NH2	ARG	E	134	88.410	16.938	82.866	1.00	99.33	E
ATOM	8353	C	ARG	E	134	84.399	16.421	76.871	1.00	99.10	E
ATOM	8354	O	ARG	E	134	83.615	16.149	77.786	1.00	100.13	E
ATOM	8355	N	ARG	E	135	84.183	16.077	75.606	1.00	101.44	E
ATOM	8356	CA	ARG	E	135	82.954	15.404	75.209	1.00	101.64	E
ATOM	8357	CB	ARG	E	135	82.405	16.077	73.955	1.00	101.47	E
ATOM	8358	CG	ARG	E	135	83.232	15.842	72.712	1.00	99.48	E
ATOM	8359	CD	ARG	E	135	82.414	15.023	71.762	1.00	101.08	E
ATOM	8360	NE	ARG	E	135	81.112	15.649	71.587	1.00	99.91	E
ATOM	8361	CZ	ARG	E	135	80.032	15.017	71.152	1.00	99.63	E



ATOM	8362	NH1	ARG	E	135	78.890	15.678	71.027	1.00101.44	E
ATOM	8363	NH2	ARG	E	135	80.090	13.726	70.853	1.00 99.66	E
ATOM	8364	C	ARG	E	135	83.025	13.902	74.978	1.00101.20	E
ATOM	8365	O	ARG	E	135	83.717	13.437	74.075	1.00101.89	E
ATOM	8366	N	SER	E	136	82.296	13.153	75.802	1.00100.13	E
ATOM	8367	CA	SER	E	136	82.230	11.700	75.678	1.00100.94	E
ATOM	8368	CB	SER	E	136	82.123	11.037	77.059	1.00100.33	E
ATOM	8369	OG	SER	E	136	83.346	11.115	77.775	1.00 99.88	E
ATOM	8370	C	SER	E	136	80.988	11.374	74.847	1.00102.00	E
ATOM	8371	O	SER	E	136	80.686	12.066	73.872	1.00101.18	E
ATOM	8372	N	ALA	E	137	80.274	10.321	75.229	1.00103.10	E
ATOM	8373	CA	ALA	E	137	79.058	9.932	74.525	1.00105.11	E
ATOM	8374	CB	ALA	E	137	79.166	8.490	74.049	1.00103.80	E
ATOM	8375	C	ALA	E	137	77.895	10.084	75.498	1.00106.97	E
ATOM	8376	O	ALA	E	137	76.781	9.619	75.242	1.00107.91	E
ATOM	8377	N	ASN	E	138	78.177	10.749	76.617	1.00107.06	E
ATOM	8378	CA	ASN	E	138	77.190	10.970	77.665	1.00106.52	E
ATOM	8379	CB	ASN	E	138	76.861	9.640	78.356	1.00107.20	E
ATOM	8380	CG	ASN	E	138	78.108	8.826	78.699	1.00106.89	E
ATOM	8381	OD1	ASN	E	138	79.019	9.295	79.395	1.00102.98	E
ATOM	8382	ND2	ASN	E	138	78.146	7.593	78.208	1.00105.22	E
ATOM	8383	C	ASN	E	138	77.643	11.977	78.719	1.00104.99	E
ATOM	8384	O	ASN	E	138	76.824	12.534	79.448	1.00103.13	E
ATOM	8385	N	SER	E	139	78.944	12.228	78.789	1.00104.04	E
ATOM	8386	CA	SER	E	139	79.458	13.137	79.802	1.00102.32	E
ATOM	8387	CB	SER	E	139	80.227	12.326	80.848	1.00102.39	E
ATOM	8388	OG	SER	E	139	79.468	11.202	81.265	1.00104.25	E
ATOM	8389	C	SER	E	139	80.329	14.296	79.316	1.00100.91	E
ATOM	8390	O	SER	E	139	81.551	14.275	79.493	1.00101.38	E
ATOM	8391	N	LEU	E	140	79.702	15.305	78.711	1.00 97.48	E
ATOM	8392	CA	LEU	E	140	80.418	16.489	78.240	1.00 91.39	E
ATOM	8393	CB	LEU	E	140	79.530	17.298	77.301	1.00 89.73	E
ATOM	8394	CG	LEU	E	140	80.225	18.400	76.501	1.00 91.43	E
ATOM	8395	CD1	LEU	E	140	79.189	19.146	75.669	1.00 89.37	E
ATOM	8396	CD2	LEU	E	140	80.952	19.352	77.441	1.00 93.09	E
ATOM	8397	C	LEU	E	140	80.734	17.313	79.491	1.00 88.57	E
ATOM	8398	O	LEU	E	140	79.837	17.651	80.260	1.00 91.20	E
ATOM	8399	N	THR	E	141	81.998	17.655	79.688	1.00 84.25	E
ATOM	8400	CA	THR	E	141	82.381	18.388	80.884	1.00 81.72	E
ATOM	8401	CB	THR	E	141	83.426	17.569	81.687	1.00 81.11	E
ATOM	8402	OG1	THR	E	141	82.877	16.283	82.005	1.00 78.08	E
ATOM	8403	CG2	THR	E	141	83.812	18.291	82.985	1.00 82.28	E
ATOM	8404	C	THR	E	141	82.915	19.807	80.683	1.00 81.01	E
ATOM	8405	O	THR	E	141	84.119	19.999	80.473	1.00 81.29	E
ATOM	8406	N	LEU	E	142	82.021	20.794	80.771	1.00 77.33	E
ATOM	8407	CA	LEU	E	142	82.408	22.200	80.633	1.00 73.34	E
ATOM	8408	CB	LEU	E	142	81.257	23.129	81.034	1.00 66.84	E
ATOM	8409	CG	LEU	E	142	79.865	23.111	80.376	1.00 70.30	E
ATOM	8410	CD1	LEU	E	142	79.897	23.800	79.028	1.00 66.49	E
ATOM	8411	CD2	LEU	E	142	79.350	21.682	80.265	1.00 67.38	E
ATOM	8412	C	LEU	E	142	83.585	22.425	81.584	1.00 73.42	E
ATOM	8413	O	LEU	E	142	83.553	21.991	82.734	1.00 72.01	E
ATOM	8414	N	ILE	E	143	84.627	23.091	81.106	1.00 74.59	E
ATOM	8415	CA	ILE	E	143	85.801	23.340	81.936	1.00 74.87	E
ATOM	8416	CB	ILE	E	143	86.975	22.436	81.493	1.00 75.32	E
ATOM	8417	CG2	ILE	E	143	86.905	22.206	80.001	1.00 76.40	E
ATOM	8418	CG1	ILE	E	143	88.316	23.047	81.907	1.00 72.09	E
ATOM	8419	CD1	ILE	E	143	88.549	23.068	83.402	1.00 78.40	E



ATOM	8420	C	ILE	E	143	86.218	24.803	81.879	1.00	74.98	E
ATOM	8421	O	ILE	E	143	86.581	25.316	80.824	1.00	76.39	E
ATOM	8422	N	ASN	E	144	86.167	25.464	83.031	1.00	73.35	E
ATOM	8423	CA	ASN	E	144	86.516	26.877	83.140	1.00	71.60	E
ATOM	8424	CB	ASN	E	144	85.314	27.658	83.676	1.00	68.98	E
ATOM	8425	CG	ASN	E	144	85.647	29.088	84.017	1.00	68.58	E
ATOM	8426	OD1	ASN	E	144	86.716	29.590	83.669	1.00	67.82	E
ATOM	8427	ND2	ASN	E	144	84.723	29.761	84.699	1.00	66.54	E
ATOM	8428	C	ASN	E	144	87.731	27.098	84.033	1.00	70.36	E
ATOM	8429	O	ASN	E	144	87.678	26.868	85.237	1.00	70.48	E
ATOM	8430	N	PRO	E	145	88.849	27.547	83.440	1.00	70.94	E
ATOM	8431	CD	PRO	E	145	89.052	27.526	81.977	1.00	71.02	E
ATOM	8432	CA	PRO	E	145	90.118	27.816	84.129	1.00	70.41	E
ATOM	8433	CB	PRO	E	145	91.150	27.442	83.079	1.00	70.45	E
ATOM	8434	CG	PRO	E	145	90.496	27.977	81.829	1.00	71.57	E
ATOM	8435	C	PRO	E	145	90.295	29.258	84.588	1.00	69.07	E
ATOM	8436	O	PRO	E	145	91.235	29.570	85.318	1.00	71.53	E
ATOM	8437	N	THR	E	146	89.402	30.136	84.148	1.00	66.19	E
ATOM	8438	CA	THR	E	146	89.472	31.549	84.510	1.00	61.24	E
ATOM	8439	CB	THR	E	146	88.520	32.361	83.641	1.00	59.37	E
ATOM	8440	OG1	THR	E	146	87.252	32.462	84.291	1.00	51.21	E
ATOM	8441	CG2	THR	E	146	88.321	31.672	82.293	1.00	57.20	E
ATOM	8442	C	THR	E	146	89.061	31.726	85.966	1.00	61.91	E
ATOM	8443	O	THR	E	146	88.882	30.751	86.685	1.00	66.35	E
ATOM	8444	N	PRO	E	147	88.942	32.973	86.433	1.00	60.67	E
ATOM	8445	CD	PRO	E	147	89.738	34.128	85.984	1.00	62.20	E
ATOM	8446	CA	PRO	E	147	88.535	33.161	87.827	1.00	58.61	E
ATOM	8447	CB	PRO	E	147	89.584	34.120	88.349	1.00	60.83	E
ATOM	8448	CG	PRO	E	147	89.695	35.061	87.202	1.00	62.62	E
ATOM	8449	C	PRO	E	147	87.128	33.752	87.925	1.00	55.62	E
ATOM	8450	O	PRO	E	147	86.787	34.388	88.921	1.00	53.78	E
ATOM	8451	N	TYR	E	148	86.322	33.546	86.886	1.00	54.39	E
ATOM	8452	CA	TYR	E	148	84.952	34.061	86.862	1.00	55.56	E
ATOM	8453	CB	TYR	E	148	84.749	35.068	85.726	1.00	54.28	E
ATOM	8454	CG	TYR	E	148	85.758	36.172	85.657	1.00	58.80	E
ATOM	8455	CD1	TYR	E	148	87.038	35.948	85.148	1.00	58.71	E
ATOM	8456	CE1	TYR	E	148	87.975	36.976	85.093	1.00	59.11	E
ATOM	8457	CD2	TYR	E	148	85.439	37.450	86.105	1.00	62.41	E
ATOM	8458	CE2	TYR	E	148	86.370	38.486	86.055	1.00	62.49	E
ATOM	8459	CZ	TYR	E	148	87.634	38.241	85.552	1.00	61.63	E
ATOM	8460	OH	TYR	E	148	88.557	39.262	85.549	1.00	69.01	E
ATOM	8461	C	TYR	E	148	83.917	32.954	86.665	1.00	54.44	E
ATOM	8462	O	TYR	E	148	84.180	31.946	86.005	1.00	55.52	E
ATOM	8463	N	TYR	E	149	82.730	33.150	87.227	1.00	48.91	E
ATOM	8464	CA	TYR	E	149	81.683	32.166	87.053	1.00	45.60	E
ATOM	8465	CB	TYR	E	149	80.530	32.406	88.044	1.00	43.27	E
ATOM	8466	CG	TYR	E	149	80.707	31.732	89.380	1.00	43.34	E
ATOM	8467	CD1	TYR	E	149	81.479	32.310	90.383	1.00	46.33	E
ATOM	8468	CE1	TYR	E	149	81.688	31.654	91.606	1.00	45.08	E
ATOM	8469	CD2	TYR	E	149	80.140	30.483	89.629	1.00	49.19	E
ATOM	8470	CE2	TYR	E	149	80.344	29.816	90.852	1.00	44.11	E
ATOM	8471	CZ	TYR	E	149	81.117	30.405	91.832	1.00	42.23	E
ATOM	8472	OH	TYR	E	149	81.316	29.755	93.032	1.00	37.45	E
ATOM	8473	C	TYR	E	149	81.180	32.283	85.612	1.00	43.17	E
ATOM	8474	O	TYR	E	149	80.794	33.360	85.163	1.00	44.66	E
ATOM	8475	N	LEU	E	150	81.183	31.175	84.884	1.00	38.35	E
ATOM	8476	CA	LEU	E	150	80.712	31.217	83.518	1.00	34.91	E
ATOM	8477	CB	LEU	E	150	81.624	30.388	82.602	1.00	35.61	E



ATOM	8478	CG	LEU	E	150	83.083	30.868	82.453	1.00	43.21	E
ATOM	8479	CD1	LEU	E	150	83.796	29.992	81.450	1.00	47.59	E
ATOM	8480	CD2	LEU	E	150	83.141	32.321	81.980	1.00	41.17	E
ATOM	8481	C	LEU	E	150	79.291	30.721	83.431	1.00	35.54	E
ATOM	8482	O	LEU	E	150	78.985	29.571	83.763	1.00	35.91	E
ATOM	8483	N	THR	E	151	78.406	31.604	82.999	1.00	35.55	E
ATOM	8484	CA	THR	E	151	77.019	31.225	82.854	1.00	38.94	E
ATOM	8485	CB	THR	E	151	76.059	32.399	83.192	1.00	38.59	E
ATOM	8486	OG1	THR	E	151	76.294	32.849	84.531	1.00	36.43	E
ATOM	8487	CG2	THR	E	151	74.606	31.947	83.078	1.00	39.58	E
ATOM	8488	C	THR	E	151	76.835	30.800	81.405	1.00	43.18	E
ATOM	8489	O	THR	E	151	76.417	31.591	80.561	1.00	47.17	E
ATOM	8490	N	VAL	E	152	77.179	29.549	81.124	1.00	45.93	E
ATOM	8491	CA	VAL	E	152	77.052	28.981	79.789	1.00	49.06	E
ATOM	8492	CB	VAL	E	152	77.826	27.652	79.676	1.00	53.34	E
ATOM	8493	CG1	VAL	E	152	77.501	26.972	78.362	1.00	51.19	E
ATOM	8494	CG2	VAL	E	152	79.327	27.904	79.796	1.00	49.69	E
ATOM	8495	C	VAL	E	152	75.595	28.703	79.448	1.00	51.18	E
ATOM	8496	O	VAL	E	152	74.922	27.954	80.146	1.00	53.77	E
ATOM	8497	N	THR	E	153	75.121	29.315	78.372	1.00	54.28	E
ATOM	8498	CA	THR	E	153	73.754	29.129	77.913	1.00	58.13	E
ATOM	8499	CB	THR	E	153	72.910	30.389	78.208	1.00	57.51	E
ATOM	8500	OG1	THR	E	153	71.546	30.185	77.796	1.00	55.66	E
ATOM	8501	CG2	THR	E	153	73.498	31.589	77.487	1.00	55.49	E
ATOM	8502	C	THR	E	153	73.785	28.842	76.400	1.00	62.76	E
ATOM	8503	O	THR	E	153	74.827	29.006	75.744	1.00	61.22	E
ATOM	8504	N	GLU	E	154	72.646	28.408	75.858	1.00	66.49	E
ATOM	8505	CA	GLU	E	154	72.517	28.069	74.438	1.00	68.76	E
ATOM	8506	CB	GLU	E	154	72.501	29.333	73.578	1.00	66.26	E
ATOM	8507	CG	GLU	E	154	71.261	30.172	73.775	1.00	72.22	E
ATOM	8508	CD	GLU	E	154	71.010	31.117	72.619	1.00	78.23	E
ATOM	8509	OE1	GLU	E	154	70.010	31.874	72.661	1.00	78.16	E
ATOM	8510	OE2	GLU	E	154	71.813	31.096	71.662	1.00	84.45	E
ATOM	8511	C	GLU	E	154	73.629	27.135	73.974	1.00	71.00	E
ATOM	8512	O	GLU	E	154	74.212	27.315	72.904	1.00	72.26	E
ATOM	8513	N	LEU	E	155	73.917	26.133	74.796	1.00	73.04	E
ATOM	8514	CA	LEU	E	155	74.947	25.150	74.492	1.00	75.03	E
ATOM	8515	CB	LEU	E	155	75.376	24.425	75.768	1.00	69.28	E
ATOM	8516	CG	LEU	E	155	76.563	23.472	75.659	1.00	64.86	E
ATOM	8517	CD1	LEU	E	155	77.823	24.263	75.323	1.00	64.88	E
ATOM	8518	CD2	LEU	E	155	76.740	22.732	76.971	1.00	63.06	E
ATOM	8519	C	LEU	E	155	74.370	24.143	73.510	1.00	80.05	E
ATOM	8520	O	LEU	E	155	73.184	23.815	73.575	1.00	79.70	E
ATOM	8521	N	ASN	E	156	75.207	23.645	72.605	1.00	85.84	E
ATOM	8522	CA	ASN	E	156	74.748	22.677	71.617	1.00	89.34	E
ATOM	8523	CB	ASN	E	156	74.198	23.415	70.406	1.00	87.22	E
ATOM	8524	CG	ASN	E	156	73.216	24.489	70.796	1.00	90.32	E
ATOM	8525	OD1	ASN	E	156	72.145	24.198	71.324	1.00	93.80	E
ATOM	8526	ND2	ASN	E	156	73.581	25.745	70.559	1.00	92.39	E
ATOM	8527	C	ASN	E	156	75.855	21.729	71.185	1.00	92.87	E
ATOM	8528	O	ASN	E	156	76.995	22.148	70.966	1.00	91.78	E
ATOM	8529	N	ALA	E	157	75.506	20.448	71.079	1.00	97.29	E
ATOM	8530	CA	ALA	E	157	76.447	19.414	70.659	1.00	101.18	E
ATOM	8531	CB	ALA	E	157	75.943	18.043	71.095	1.00	101.13	E
ATOM	8532	C	ALA	E	157	76.549	19.480	69.139	1.00	104.35	E
ATOM	8533	O	ALA	E	157	76.729	18.465	68.462	1.00	105.98	E
ATOM	8534	N	GLY	E	158	76.424	20.698	68.619	1.00	106.48	E
ATOM	8535	CA	GLY	E	158	76.485	20.924	67.190	1.00	107.57	E



ATOM	8536	C	GLY	E	158	75.101	21.234	66.663	1.00109.34	E
ATOM	8537	O	GLY	E	158	74.864	22.310	66.110	1.00109.40	E
ATOM	8538	N	THR	E	159	74.186	20.284	66.847	1.00111.07	E
ATOM	8539	CA	THR	E	159	72.804	20.423	66.397	1.00112.63	E
ATOM	8540	CB	THR	E	159	72.420	19.317	65.400	1.00113.41	E
ATOM	8541	OG1	THR	E	159	72.497	18.045	66.055	1.00114.77	E
ATOM	8542	CG2	THR	E	159	73.362	19.319	64.202	1.00115.94	E
ATOM	8543	C	THR	E	159	71.892	20.278	67.600	1.00113.37	E
ATOM	8544	O	THR	E	159	70.950	21.050	67.781	1.00113.17	E
ATOM	8545	N	ARG	E	160	72.186	19.269	68.414	1.00114.32	E
ATOM	8546	CA	ARG	E	160	71.412	18.993	69.612	1.00115.70	E
ATOM	8547	CB	ARG	E	160	71.904	17.697	70.263	1.00120.12	E
ATOM	8548	CG	ARG	E	160	71.060	17.210	71.440	1.00127.73	E
ATOM	8549	CD	ARG	E	160	69.765	16.535	70.973	1.00132.71	E
ATOM	8550	NE	ARG	E	160	69.083	15.831	72.057	1.00137.48	E
ATOM	8551	CZ	ARG	E	160	68.282	16.409	72.949	1.00137.60	E
ATOM	8552	NH1	ARG	E	160	68.042	17.715	72.889	1.00139.24	E
ATOM	8553	NH2	ARG	E	160	67.742	15.683	73.921	1.00136.81	E
ATOM	8554	C	ARG	E	160	71.564	20.150	70.596	1.00113.60	E
ATOM	8555	O	ARG	E	160	72.660	20.680	70.787	1.00113.52	E
ATOM	8556	N	VAL	E	161	70.455	20.542	71.210	1.00110.19	E
ATOM	8557	CA	VAL	E	161	70.469	21.621	72.188	1.00107.35	E
ATOM	8558	CB	VAL	E	161	69.206	22.507	72.066	1.00109.21	E
ATOM	8559	CG1	VAL	E	161	67.946	21.664	72.276	1.00108.93	E
ATOM	8560	CG2	VAL	E	161	69.271	23.646	73.075	1.00107.68	E
ATOM	8561	C	VAL	E	161	70.532	21.017	73.589	1.00104.33	E
ATOM	8562	O	VAL	E	161	69.769	20.108	73.923	1.00104.97	E
ATOM	8563	N	LEU	E	162	71.441	21.522	74.412	1.00100.01	E
ATOM	8564	CA	LEU	E	162	71.586	21.004	75.766	1.00 96.80	E
ATOM	8565	CB	LEU	E	162	73.064	20.771	76.074	1.00 97.92	E
ATOM	8566	CG	LEU	E	162	73.747	19.749	75.169	1.00 98.31	E
ATOM	8567	CD1	LEU	E	162	75.191	19.552	75.610	1.00 97.42	E
ATOM	8568	CD2	LEU	E	162	72.979	18.439	75.237	1.00 98.39	E
ATOM	8569	C	LEU	E	162	70.973	21.872	76.863	1.00 93.12	E
ATOM	8570	O	LEU	E	162	70.147	22.757	76.608	1.00 92.56	E
ATOM	8571	N	GLU	E	163	71.392	21.603	78.094	1.00 87.79	E
ATOM	8572	CA	GLU	E	163	70.898	22.333	79.246	1.00 82.65	E
ATOM	8573	CB	GLU	E	163	70.487	21.341	80.332	1.00 85.22	E
ATOM	8574	CG	GLU	E	163	69.640	21.933	81.440	1.00 90.62	E
ATOM	8575	CD	GLU	E	163	68.706	20.907	82.053	1.00 91.02	E
ATOM	8576	OE1	GLU	E	163	67.695	20.564	81.402	1.00 89.20	E
ATOM	8577	OE2	GLU	E	163	68.987	20.436	83.178	1.00 93.62	E
ATOM	8578	C	GLU	E	163	71.974	23.293	79.756	1.00 77.13	E
ATOM	8579	O	GLU	E	163	73.156	22.933	79.861	1.00 76.00	E
ATOM	8580	N	ASN	E	164	71.554	24.519	80.060	1.00 68.76	E
ATOM	8581	CA	ASN	E	164	72.458	25.561	80.537	1.00 62.46	E
ATOM	8582	CB	ASN	E	164	71.651	26.757	81.010	1.00 62.03	E
ATOM	8583	CG	ASN	E	164	70.605	27.165	80.012	1.00 66.90	E
ATOM	8584	OD1	ASN	E	164	70.921	27.669	78.934	1.00 68.02	E
ATOM	8585	ND2	ASN	E	164	69.342	26.938	80.356	1.00 73.37	E
ATOM	8586	C	ASN	E	164	73.371	25.097	81.658	1.00 58.94	E
ATOM	8587	O	ASN	E	164	73.071	24.145	82.371	1.00 60.17	E
ATOM	8588	N	ALA	E	165	74.491	25.780	81.826	1.00 54.91	E
ATOM	8589	CA	ALA	E	165	75.410	25.399	82.877	1.00 53.53	E
ATOM	8590	CB	ALA	E	165	76.477	24.474	82.332	1.00 54.95	E
ATOM	8591	C	ALA	E	165	76.048	26.614	83.498	1.00 53.05	E
ATOM	8592	O	ALA	E	165	76.126	27.676	82.879	1.00 52.33	E
ATOM	8593	N	LEU	E	166	76.478	26.446	84.743	1.00 49.24	E



ATOM	8594	CA	LEU	E	166	77.131	27.503	85.485	1.00	44.72	E
ATOM	8595	CB	LEU	E	166	76.327	27.856	86.738	1.00	39.66	E
ATOM	8596	CG	LEU	E	166	76.968	28.874	87.688	1.00	45.21	E
ATOM	8597	CD1	LEU	E	166	77.152	30.220	86.972	1.00	39.91	E
ATOM	8598	CD2	LEU	E	166	76.094	29.044	88.909	1.00	40.37	E
ATOM	8599	C	LEU	E	166	78.472	26.907	85.854	1.00	42.70	E
ATOM	8600	O	LEU	E	166	78.556	26.042	86.709	1.00	43.32	E
ATOM	8601	N	VAL	E	167	79.530	27.355	85.196	1.00	43.34	E
ATOM	8602	CA	VAL	E	167	80.832	26.788	85.487	1.00	43.55	E
ATOM	8603	CB	VAL	E	167	81.638	26.516	84.215	1.00	42.61	E
ATOM	8604	CG1	VAL	E	167	82.873	25.711	84.561	1.00	45.25	E
ATOM	8605	CG2	VAL	E	167	80.777	25.771	83.201	1.00	45.20	E
ATOM	8606	C	VAL	E	167	81.662	27.654	86.392	1.00	45.84	E
ATOM	8607	O	VAL	E	167	82.086	28.748	86.020	1.00	48.46	E
ATOM	8608	N	PRO	E	168	81.920	27.157	87.602	1.00	47.47	E
ATOM	8609	CD	PRO	E	168	81.459	25.828	88.036	1.00	43.22	E
ATOM	8610	CA	PRO	E	168	82.702	27.803	88.656	1.00	49.69	E
ATOM	8611	CB	PRO	E	168	82.636	26.790	89.790	1.00	49.05	E
ATOM	8612	CG	PRO	E	168	82.490	25.478	89.065	1.00	48.13	E
ATOM	8613	C	PRO	E	168	84.138	28.130	88.261	1.00	52.62	E
ATOM	8614	O	PRO	E	168	84.733	27.451	87.431	1.00	53.52	E
ATOM	8615	N	PRO	E	169	84.713	29.180	88.866	1.00	56.85	E
ATOM	8616	CD	PRO	E	169	84.038	30.057	89.838	1.00	59.48	E
ATOM	8617	CA	PRO	E	169	86.083	29.645	88.622	1.00	59.66	E
ATOM	8618	CB	PRO	E	169	86.260	30.756	89.654	1.00	60.30	E
ATOM	8619	CG	PRO	E	169	84.890	31.315	89.775	1.00	62.59	E
ATOM	8620	C	PRO	E	169	87.089	28.527	88.841	1.00	61.57	E
ATOM	8621	O	PRO	E	169	86.972	27.772	89.806	1.00	65.74	E
ATOM	8622	N	MET	E	170	88.077	28.427	87.958	1.00	61.17	E
ATOM	8623	CA	MET	E	170	89.096	27.396	88.080	1.00	58.16	E
ATOM	8624	CB	MET	E	170	90.132	27.835	89.105	1.00	58.25	E
ATOM	8625	CG	MET	E	170	90.950	29.007	88.618	1.00	70.37	E
ATOM	8626	SD	MET	E	170	91.910	29.829	89.892	1.00	83.55	E
ATOM	8627	CE	MET	E	170	90.978	31.381	90.036	1.00	84.38	E
ATOM	8628	C	MET	E	170	88.465	26.071	88.481	1.00	56.84	E
ATOM	8629	O	MET	E	170	89.014	25.323	89.288	1.00	56.41	E
ATOM	8630	N	GLY	E	171	87.299	25.799	87.907	1.00	54.79	E
ATOM	8631	CA	GLY	E	171	86.591	24.575	88.200	1.00	57.47	E
ATOM	8632	C	GLY	E	171	85.943	24.042	86.944	1.00	62.52	E
ATOM	8633	O	GLY	E	171	86.310	24.442	85.840	1.00	64.05	E
ATOM	8634	N	GLU	E	172	84.970	23.151	87.103	1.00	65.70	E
ATOM	8635	CA	GLU	E	172	84.302	22.560	85.955	1.00	69.00	E
ATOM	8636	CB	GLU	E	172	85.222	21.511	85.330	1.00	75.52	E
ATOM	8637	CG	GLU	E	172	85.828	20.545	86.341	1.00	79.82	E
ATOM	8638	CD	GLU	E	172	86.952	19.721	85.744	1.00	85.82	E
ATOM	8639	OE1	GLU	E	172	86.673	18.932	84.814	1.00	85.82	E
ATOM	8640	OE2	GLU	E	172	88.112	19.868	86.198	1.00	87.13	E
ATOM	8641	C	GLU	E	172	82.955	21.937	86.293	1.00	67.75	E
ATOM	8642	O	GLU	E	172	82.654	21.667	87.448	1.00	68.63	E
ATOM	8643	N	SER	E	173	82.154	21.702	85.262	1.00	67.64	E
ATOM	8644	CA	SER	E	173	80.830	21.121	85.417	1.00	70.11	E
ATOM	8645	CB	SER	E	173	79.778	22.230	85.407	1.00	67.59	E
ATOM	8646	OG	SER	E	173	80.298	23.417	85.980	1.00	71.50	E
ATOM	8647	C	SER	E	173	80.570	20.177	84.248	1.00	73.57	E
ATOM	8648	O	SER	E	173	81.030	20.426	83.130	1.00	72.53	E
ATOM	8649	N	ALA	E	174	79.829	19.103	84.496	1.00	76.59	E
ATOM	8650	CA	ALA	E	174	79.528	18.158	83.435	1.00	78.85	E
ATOM	8651	CB	ALA	E	174	80.004	16.759	83.835	1.00	76.70	E



ATOM	8652	C	ALA	E	174	78.042	18.129	83.101	1.00	80.41	E
ATOM	8653	O	ALA	E	174	77.217	17.789	83.944	1.00	82.68	E
ATOM	8654	N	VAL	E	175	77.704	18.509	81.876	1.00	83.44	E
ATOM	8655	CA	VAL	E	175	76.323	18.473	81.417	1.00	90.29	E
ATOM	8656	CB	VAL	E	175	76.018	19.623	80.430	1.00	91.72	E
ATOM	8657	CG1	VAL	E	175	74.662	19.388	79.756	1.00	87.34	E
ATOM	8658	CG2	VAL	E	175	76.027	20.969	81.142	1.00	93.34	E
ATOM	8659	C	VAL	E	175	76.115	17.147	80.699	1.00	95.14	E
ATOM	8660	O	VAL	E	175	76.955	16.740	79.897	1.00	96.50	E
ATOM	8661	N	LYS	E	176	75.005	16.473	80.998	1.00	97.88	E
ATOM	8662	CA	LYS	E	176	74.719	15.180	80.382	1.00	101.17	E
ATOM	8663	CB	LYS	E	176	73.330	14.668	80.777	1.00	99.65	E
ATOM	8664	CG	LYS	E	176	73.189	14.266	82.252	1.00	101.69	E
ATOM	8665	CD	LYS	E	176	73.270	15.474	83.198	1.00	100.25	E
ATOM	8666	CE	LYS	E	176	72.853	15.114	84.629	1.00	92.38	E
ATOM	8667	NZ	LYS	E	176	73.712	14.037	85.201	1.00	84.47	E
ATOM	8668	C	LYS	E	176	74.798	15.279	78.857	1.00	105.86	E
ATOM	8669	O	LYS	E	176	74.010	15.985	78.230	1.00	106.00	E
ATOM	8670	N	LEU	E	177	75.761	14.569	78.271	1.00	109.97	E
ATOM	8671	CA	LEU	E	177	75.976	14.532	76.821	1.00	113.55	E
ATOM	8672	CB	LEU	E	177	77.442	14.180	76.563	1.00	111.13	E
ATOM	8673	CG	LEU	E	177	78.005	14.236	75.140	1.00	110.68	E
ATOM	8674	CD1	LEU	E	177	77.402	15.402	74.356	1.00	109.76	E
ATOM	8675	CD2	LEU	E	177	79.528	14.389	75.214	1.00	108.19	E
ATOM	8676	C	LEU	E	177	75.022	13.495	76.207	1.00	116.96	E
ATOM	8677	O	LEU	E	177	75.188	12.289	76.394	1.00	117.37	E
ATOM	8678	N	PRO	E	178	74.016	13.969	75.448	1.00	119.88	E
ATOM	8679	CD	PRO	E	178	73.902	15.386	75.058	1.00	120.42	E
ATOM	8680	CA	PRO	E	178	72.975	13.183	74.775	1.00	122.91	E
ATOM	8681	CB	PRO	E	178	72.077	14.260	74.184	1.00	120.33	E
ATOM	8682	CG	PRO	E	178	73.054	15.305	73.805	1.00	122.24	E
ATOM	8683	C	PRO	E	178	73.379	12.150	73.722	1.00	126.75	E
ATOM	8684	O	PRO	E	178	72.601	11.236	73.422	1.00	128.10	E
ATOM	8685	N	SER	E	179	74.575	12.292	73.158	1.00	128.80	E
ATOM	8686	CA	SER	E	179	75.077	11.383	72.116	1.00	129.28	E
ATOM	8687	CB	SER	E	179	74.844	9.911	72.502	1.00	129.66	E
ATOM	8688	OG	SER	E	179	75.544	9.038	71.628	1.00	128.71	E
ATOM	8689	C	SER	E	179	74.528	11.675	70.711	1.00	128.87	E
ATOM	8690	O	SER	E	179	75.050	11.164	69.707	1.00	128.52	E
ATOM	8691	N	ASP	E	180	73.462	12.477	70.649	1.00	127.78	E
ATOM	8692	CA	ASP	E	180	72.880	12.925	69.372	1.00	125.71	E
ATOM	8693	CB	ASP	E	180	71.479	13.522	69.588	1.00	124.59	E
ATOM	8694	CG	ASP	E	180	70.483	12.516	70.119	1.00	123.01	E
ATOM	8695	OD1	ASP	E	180	69.321	12.908	70.394	1.00	122.29	E
ATOM	8696	OD2	ASP	E	180	70.851	11.332	70.252	1.00	121.06	E
ATOM	8697	C	ASP	E	180	73.865	14.034	69.007	1.00	124.59	E
ATOM	8698	O	ASP	E	180	73.555	15.019	68.362	1.00	122.89	E
ATOM	8699	N	ALA	E	181	75.073	13.791	69.492	1.00	124.55	E
ATOM	8700	CA	ALA	E	181	76.270	14.608	69.423	1.00	124.38	E
ATOM	8701	CB	ALA	E	181	77.423	13.771	69.866	1.00	123.55	E
ATOM	8702	C	ALA	E	181	76.653	15.298	68.125	1.00	124.78	E
ATOM	8703	O	ALA	E	181	75.821	15.684	67.298	1.00	123.76	E
ATOM	8704	N	GLY	E	182	77.967	15.498	68.043	1.00	125.49	E
ATOM	8705	CA	GLY	E	182	78.650	16.132	66.935	1.00	127.02	E
ATOM	8706	C	GLY	E	182	80.070	16.339	67.429	1.00	128.13	E
ATOM	8707	O	GLY	E	182	80.868	15.401	67.462	1.00	129.50	E
ATOM	8708	N	SER	E	183	80.354	17.565	67.842	1.00	127.43	E
ATOM	8709	CA	SER	E	183	81.648	17.974	68.359	1.00	125.46	E



ATOM	8710	CB	SER	E	183	82.801	17.262	67.658	1.00125.67	E
ATOM	8711	OG	SER	E	183	83.949	17.259	68.489	1.00126.90	E
ATOM	8712	C	SER	E	183	81.659	19.442	68.001	1.00123.66	E
ATOM	8713	O	SER	E	183	82.537	20.209	68.404	1.00122.44	E
ATOM	8714	N	ASN	E	184	80.651	19.813	67.217	1.00121.65	E
ATOM	8715	CA	ASN	E	184	80.449	21.186	66.782	1.00118.72	E
ATOM	8716	CB	ASN	E	184	79.452	21.235	65.610	1.00118.99	E
ATOM	8717	CG	ASN	E	184	79.138	22.657	65.161	1.00119.20	E
ATOM	8718	OD1	ASN	E	184	80.032	23.397	64.744	1.00119.22	E
ATOM	8719	ND2	ASN	E	184	77.865	23.045	65.249	1.00118.04	E
ATOM	8720	C	ASN	E	184	79.867	21.900	67.987	1.00115.53	E
ATOM	8721	O	ASN	E	184	78.908	22.671	67.877	1.00114.96	E
ATOM	8722	N	ILE	E	185	80.442	21.610	69.147	1.00112.17	E
ATOM	8723	CA	ILE	E	185	79.983	22.220	70.382	1.00108.97	E
ATOM	8724	CB	ILE	E	185	80.936	21.901	71.552	1.00106.93	E
ATOM	8725	CG2	ILE	E	185	80.427	22.564	72.826	1.00108.27	E
ATOM	8726	CG1	ILE	E	185	81.023	20.385	71.757	1.00102.38	E
ATOM	8727	CD1	ILE	E	185	81.884	19.970	72.925	1.00100.01	E
ATOM	8728	C	ILE	E	185	79.868	23.737	70.204	1.00106.71	E
ATOM	8729	O	ILE	E	185	80.812	24.403	69.776	1.00106.68	E
ATOM	8730	N	THR	E	186	78.694	24.269	70.522	1.00102.01	E
ATOM	8731	CA	THR	E	186	78.432	25.691	70.376	1.00 96.59	E
ATOM	8732	CB	THR	E	186	77.513	25.910	69.198	1.00 94.19	E
ATOM	8733	OG1	THR	E	186	76.413	25.000	69.289	1.00 95.20	E
ATOM	8734	CG2	THR	E	186	78.246	25.641	67.912	1.00 95.63	E
ATOM	8735	C	THR	E	186	77.806	26.288	71.629	1.00 92.99	E
ATOM	8736	O	THR	E	186	76.958	25.661	72.273	1.00 91.83	E
ATOM	8737	N	TYR	E	187	78.211	27.510	71.969	1.00 87.88	E
ATOM	8738	CA	TYR	E	187	77.698	28.140	73.176	1.00 79.80	E
ATOM	8739	CB	TYR	E	187	78.435	27.570	74.374	1.00 74.43	E
ATOM	8740	CG	TYR	E	187	79.874	28.011	74.405	1.00 68.14	E
ATOM	8741	CD1	TYR	E	187	80.229	29.268	74.885	1.00 69.19	E
ATOM	8742	CE1	TYR	E	187	81.545	29.695	74.885	1.00 67.19	E
ATOM	8743	CD2	TYR	E	187	80.878	27.189	73.925	1.00 70.36	E
ATOM	8744	CE2	TYR	E	187	82.203	27.607	73.919	1.00 70.04	E
ATOM	8745	CZ	TYR	E	187	82.526	28.861	74.402	1.00 67.80	E
ATOM	8746	OH	TYR	E	187	83.833	29.276	74.403	1.00 71.27	E
ATOM	8747	C	TYR	E	187	77.872	29.644	73.209	1.00 76.42	E
ATOM	8748	O	TYR	E	187	78.769	30.194	72.575	1.00 78.21	E
ATOM	8749	N	ARG	E	188	77.015	30.295	73.982	1.00 72.37	E
ATOM	8750	CA	ARG	E	188	77.083	31.738	74.188	1.00 67.64	E
ATOM	8751	CB	ARG	E	188	75.839	32.419	73.611	1.00 69.25	E
ATOM	8752	CG	ARG	E	188	75.546	32.047	72.166	1.00 73.45	E
ATOM	8753	CD	ARG	E	188	74.194	32.565	71.713	1.00 72.84	E
ATOM	8754	NE	ARG	E	188	74.167	34.017	71.599	1.00 79.18	E
ATOM	8755	CZ	ARG	E	188	74.839	34.707	70.683	1.00 82.45	E
ATOM	8756	NH1	ARG	E	188	75.594	34.073	69.797	1.00 83.73	E
ATOM	8757	NH2	ARG	E	188	74.750	36.031	70.647	1.00 83.44	E
ATOM	8758	C	ARG	E	188	77.086	31.830	75.719	1.00 62.29	E
ATOM	8759	O	ARG	E	188	76.856	30.819	76.390	1.00 62.83	E
ATOM	8760	N	THR	E	189	77.381	32.991	76.291	1.00 53.76	E
ATOM	8761	CA	THR	E	189	77.341	33.078	77.749	1.00 48.05	E
ATOM	8762	CB	THR	E	189	78.721	33.086	78.399	1.00 40.38	E
ATOM	8763	OG1	THR	E	189	79.297	34.388	78.272	1.00 32.65	E
ATOM	8764	CG2	THR	E	189	79.605	32.041	77.771	1.00 36.01	E
ATOM	8765	C	THR	E	189	76.624	34.331	78.190	1.00 49.51	E
ATOM	8766	O	THR	E	189	76.094	35.075	77.358	1.00 52.41	E
ATOM	8767	N	ILE	E	190	76.594	34.564	79.502	1.00 44.96	E



ATOM	8768	CA	ILE	E	190	75.914	35.734	80.019	1.00	40.50	E
ATOM	8769	CB	ILE	E	190	74.725	35.298	80.882	1.00	31.68	E
ATOM	8770	CG2	ILE	E	190	73.881	36.497	81.268	1.00	28.51	E
ATOM	8771	CG1	ILE	E	190	73.875	34.315	80.066	1.00	31.75	E
ATOM	8772	CD1	ILE	E	190	72.577	33.905	80.682	1.00	26.13	E
ATOM	8773	C	ILE	E	190	76.907	36.619	80.773	1.00	45.23	E
ATOM	8774	O	ILE	E	190	77.490	36.218	81.787	1.00	48.10	E
ATOM	8775	N	ASN	E	191	77.111	37.825	80.247	1.00	43.17	E
ATOM	8776	CA	ASN	E	191	78.052	38.768	80.832	1.00	42.56	E
ATOM	8777	CB	ASN	E	191	78.583	39.717	79.765	1.00	44.01	E
ATOM	8778	CG	ASN	E	191	77.482	40.553	79.140	1.00	46.11	E
ATOM	8779	OD1	ASN	E	191	76.658	41.165	79.837	1.00	46.43	E
ATOM	8780	ND2	ASN	E	191	77.463	40.586	77.822	1.00	46.59	E
ATOM	8781	C	ASN	E	191	77.468	39.613	81.945	1.00	41.73	E
ATOM	8782	O	ASN	E	191	76.253	39.642	82.171	1.00	43.47	E
ATOM	8783	N	ASP	E	192	78.375	40.328	82.597	1.00	34.08	E
ATOM	8784	CA	ASP	E	192	78.076	41.212	83.697	1.00	30.90	E
ATOM	8785	CB	ASP	E	192	79.258	42.150	83.938	1.00	33.04	E
ATOM	8786	CG	ASP	E	192	80.517	41.422	84.397	1.00	37.46	E
ATOM	8787	OD1	ASP	E	192	81.475	42.114	84.790	1.00	35.45	E
ATOM	8788	OD2	ASP	E	192	80.556	40.174	84.369	1.00	41.56	E
ATOM	8789	C	ASP	E	192	76.836	42.059	83.500	1.00	34.39	E
ATOM	8790	O	ASP	E	192	76.302	42.602	84.465	1.00	36.04	E
ATOM	8791	N	TYR	E	193	76.367	42.188	82.265	1.00	36.79	E
ATOM	8792	CA	TYR	E	193	75.196	43.024	82.021	1.00	39.38	E
ATOM	8793	CB	TYR	E	193	75.481	44.011	80.895	1.00	39.88	E
ATOM	8794	CG	TYR	E	193	76.807	44.676	81.098	1.00	43.20	E
ATOM	8795	CD1	TYR	E	193	77.919	44.283	80.363	1.00	44.07	E
ATOM	8796	CE1	TYR	E	193	79.173	44.832	80.612	1.00	49.04	E
ATOM	8797	CD2	TYR	E	193	76.977	45.641	82.094	1.00	45.49	E
ATOM	8798	CE2	TYR	E	193	78.226	46.197	82.354	1.00	47.91	E
ATOM	8799	CZ	TYR	E	193	79.322	45.789	81.608	1.00	48.45	E
ATOM	8800	OH	TYR	E	193	80.559	46.346	81.851	1.00	49.86	E
ATOM	8801	C	TYR	E	193	73.999	42.185	81.703	1.00	39.19	E
ATOM	8802	O	TYR	E	193	72.972	42.682	81.238	1.00	39.41	E
ATOM	8803	N	GLY	E	194	74.147	40.898	81.975	1.00	40.01	E
ATOM	8804	CA	GLY	E	194	73.064	39.970	81.746	1.00	44.70	E
ATOM	8805	C	GLY	E	194	72.773	39.937	80.278	1.00	46.02	E
ATOM	8806	O	GLY	E	194	71.633	39.719	79.858	1.00	40.25	E
ATOM	8807	N	ALA	E	195	73.833	40.170	79.508	1.00	52.12	E
ATOM	8808	CA	ALA	E	195	73.760	40.184	78.056	1.00	55.14	E
ATOM	8809	CB	ALA	E	195	74.410	41.457	77.528	1.00	57.76	E
ATOM	8810	C	ALA	E	195	74.455	38.946	77.482	1.00	55.29	E
ATOM	8811	O	ALA	E	195	75.464	38.486	78.019	1.00	49.52	E
ATOM	8812	N	LEU	E	196	73.889	38.407	76.402	1.00	59.02	E
ATOM	8813	CA	LEU	E	196	74.437	37.227	75.738	1.00	60.62	E
ATOM	8814	CB	LEU	E	196	73.426	36.642	74.751	1.00	60.51	E
ATOM	8815	CG	LEU	E	196	72.222	35.873	75.299	1.00	65.69	E
ATOM	8816	CD1	LEU	E	196	71.244	35.532	74.174	1.00	62.28	E
ATOM	8817	CD2	LEU	E	196	72.714	34.610	75.982	1.00	64.87	E
ATOM	8818	C	LEU	E	196	75.697	37.585	74.973	1.00	62.63	E
ATOM	8819	O	LEU	E	196	75.699	38.509	74.164	1.00	66.96	E
ATOM	8820	N	THR	E	197	76.779	36.867	75.233	1.00	63.16	E
ATOM	8821	CA	THR	E	197	78.005	37.138	74.514	1.00	62.75	E
ATOM	8822	CB	THR	E	197	79.230	36.514	75.208	1.00	61.23	E
ATOM	8823	OG1	THR	E	197	79.143	35.081	75.165	1.00	57.40	E
ATOM	8824	CG2	THR	E	197	79.304	36.995	76.648	1.00	58.08	E
ATOM	8825	C	THR	E	197	77.806	36.515	73.139	1.00	66.39	E



ATOM	8826	O	THR	E	197	76.825	35.803	72.905	1.00	63.48	E
ATOM	8827	N	PRO	E	198	78.719	36.788	72.202	1.00	69.71	E
ATOM	8828	CD	PRO	E	198	79.898	37.668	72.264	1.00	69.96	E
ATOM	8829	CA	PRO	E	198	78.563	36.208	70.869	1.00	72.15	E
ATOM	8830	CB	PRO	E	198	79.535	37.028	70.033	1.00	69.88	E
ATOM	8831	CG	PRO	E	198	80.645	37.289	71.010	1.00	72.14	E
ATOM	8832	C	PRO	E	198	78.878	34.712	70.847	1.00	74.56	E
ATOM	8833	O	PRO	E	198	79.776	34.241	71.558	1.00	75.65	E
ATOM	8834	N	LYS	E	199	78.124	33.981	70.028	1.00	75.53	E
ATOM	8835	CA	LYS	E	199	78.272	32.536	69.859	1.00	74.73	E
ATOM	8836	CB	LYS	E	199	77.343	32.077	68.736	1.00	73.23	E
ATOM	8837	CG	LYS	E	199	77.467	30.631	68.310	1.00	80.01	E
ATOM	8838	CD	LYS	E	199	76.305	30.309	67.362	1.00	86.06	E
ATOM	8839	CE	LYS	E	199	76.582	29.118	66.443	1.00	90.81	E
ATOM	8840	NZ	LYS	E	199	76.745	27.832	67.166	1.00	91.20	E
ATOM	8841	C	LYS	E	199	79.714	32.154	69.545	1.00	75.13	E
ATOM	8842	O	LYS	E	199	80.340	32.744	68.672	1.00	76.16	E
ATOM	8843	N	MET	E	200	80.250	31.180	70.268	1.00	76.95	E
ATOM	8844	CA	MET	E	200	81.620	30.744	70.031	1.00	78.07	E
ATOM	8845	CB	MET	E	200	82.511	31.087	71.222	1.00	80.58	E
ATOM	8846	CG	MET	E	200	81.902	32.082	72.179	1.00	83.33	E
ATOM	8847	SD	MET	E	200	83.157	32.884	73.180	1.00	94.18	E
ATOM	8848	CE	MET	E	200	82.635	34.607	73.015	1.00	92.27	E
ATOM	8849	C	MET	E	200	81.610	29.244	69.806	1.00	77.40	E
ATOM	8850	O	MET	E	200	80.627	28.573	70.135	1.00	76.60	E
ATOM	8851	N	THR	E	201	82.703	28.720	69.254	1.00	77.22	E
ATOM	8852	CA	THR	E	201	82.798	27.293	68.967	1.00	77.48	E
ATOM	8853	CB	THR	E	201	83.500	27.038	67.611	1.00	76.20	E
ATOM	8854	OG1	THR	E	201	82.748	27.660	66.560	1.00	76.69	E
ATOM	8855	CG2	THR	E	201	83.591	25.542	67.332	1.00	71.96	E
ATOM	8856	C	THR	E	201	83.511	26.480	70.037	1.00	77.79	E
ATOM	8857	O	THR	E	201	84.582	26.855	70.517	1.00	78.02	E
ATOM	8858	N	GLY	E	202	82.900	25.356	70.394	1.00	78.70	E
ATOM	8859	CA	GLY	E	202	83.470	24.476	71.392	1.00	83.61	E
ATOM	8860	C	GLY	E	202	84.876	24.068	71.016	1.00	86.50	E
ATOM	8861	O	GLY	E	202	85.135	23.706	69.868	1.00	87.22	E
ATOM	8862	N	VAL	E	203	85.780	24.118	71.988	1.00	88.73	E
ATOM	8863	CA	VAL	E	203	87.179	23.773	71.764	1.00	91.05	E
ATOM	8864	CB	VAL	E	203	88.051	25.040	71.845	1.00	90.32	E
ATOM	8865	CG1	VAL	E	203	89.493	24.715	71.492	1.00	87.74	E
ATOM	8866	CG2	VAL	E	203	87.488	26.103	70.920	1.00	85.78	E
ATOM	8867	C	VAL	E	203	87.675	22.760	72.796	1.00	93.95	E
ATOM	8868	O	VAL	E	203	88.419	23.115	73.714	1.00	96.85	E
ATOM	8869	N	MET	E	204	87.266	21.503	72.638	1.00	95.46	E
ATOM	8870	CA	MET	E	204	87.650	20.434	73.566	1.00	98.14	E
ATOM	8871	CB	MET	E	204	87.354	19.060	72.948	1.00	101.59	E
ATOM	8872	CG	MET	E	204	85.874	18.786	72.658	1.00	105.16	E
ATOM	8873	SD	MET	E	204	85.119	19.917	71.448	1.00	112.63	E
ATOM	8874	CE	MET	E	204	85.504	19.094	69.897	1.00	110.01	E
ATOM	8875	C	MET	E	204	89.119	20.497	73.982	1.00	97.01	E
ATOM	8876	O	MET	E	204	90.001	20.657	73.148	1.00	95.27	E
ATOM	8877	N	GLU	E	205	89.377	20.380	75.280	1.00	99.01	E
ATOM	8878	CA	GLU	E	205	90.744	20.419	75.780	1.00	102.65	E
ATOM	8879	CB	GLU	E	205	90.800	20.949	77.218	1.00	105.77	E
ATOM	8880	CG	GLU	E	205	90.280	19.973	78.275	1.00	112.16	E
ATOM	8881	CD	GLU	E	205	91.278	19.734	79.407	1.00	115.73	E
ATOM	8882	OE1	GLU	E	205	90.954	18.965	80.345	1.00	116.43	E
ATOM	8883	OE2	GLU	E	205	92.385	20.313	79.356	1.00	116.20	E



ATOM	8884	C	GLU	E	205	91.305	19.012	75.746	1.00104.46	E
ATOM	8885	O	GLU	E	205	92.488	18.867	75.373	1.00104.28	E
ATOM	8886	OXT	GLU	E	205	90.553	18.079	76.112	1.00107.35	E
ATOM	8887	CB	PHE	F	1	80.812	82.422	60.648	1.00 33.92	F
ATOM	8888	CG	PHE	F	1	80.164	81.444	61.587	1.00 35.95	F
ATOM	8889	CD1	PHE	F	1	79.979	80.113	61.215	1.00 39.29	F
ATOM	8890	CD2	PHE	F	1	79.786	81.834	62.867	1.00 34.66	F
ATOM	8891	CE1	PHE	F	1	79.436	79.192	62.102	1.00 30.20	F
ATOM	8892	CE2	PHE	F	1	79.238	80.916	63.765	1.00 30.16	F
ATOM	8893	CZ	PHE	F	1	79.066	79.595	63.380	1.00 33.16	F
ATOM	8894	C	PHE	F	1	82.921	81.051	60.380	1.00 30.85	F
ATOM	8895	O	PHE	F	1	82.798	80.576	59.260	1.00 28.03	F
ATOM	8896	N	PHE	F	1	82.903	83.402	59.737	1.00 39.15	F
ATOM	8897	CA	PHE	F	1	82.354	82.424	60.714	1.00 34.90	F
ATOM	8898	N	ALA	F	2	83.561	80.428	61.359	1.00 32.93	F
ATOM	8899	CA	ALA	F	2	84.156	79.107	61.178	1.00 32.00	F
ATOM	8900	CB	ALA	F	2	85.591	79.252	60.743	1.00 22.11	F
ATOM	8901	C	ALA	F	2	84.083	78.330	62.492	1.00 32.49	F
ATOM	8902	O	ALA	F	2	83.977	78.919	63.574	1.00 33.00	F
ATOM	8903	N	CYS	F	3	84.141	77.007	62.408	1.00 30.62	F
ATOM	8904	CA	CYS	F	3	84.078	76.196	63.615	1.00 31.66	F
ATOM	8905	C	CYS	F	3	85.190	75.150	63.624	1.00 31.86	F
ATOM	8906	O	CYS	F	3	85.765	74.840	62.590	1.00 31.93	F
ATOM	8907	CB	CYS	F	3	82.730	75.497	63.709	1.00 32.29	F
ATOM	8908	SG	CYS	F	3	81.240	76.539	63.584	1.00 40.59	F
ATOM	8909	N	LYS	F	4	85.503	74.619	64.799	1.00 32.55	F
ATOM	8910	CA	LYS	F	4	86.533	73.603	64.916	1.00 35.01	F
ATOM	8911	CB	LYS	F	4	87.888	74.203	65.308	1.00 34.04	F
ATOM	8912	CG	LYS	F	4	87.932	74.783	66.712	1.00 43.93	F
ATOM	8913	CD	LYS	F	4	89.251	75.509	67.023	1.00 53.56	F
ATOM	8914	CE	LYS	F	4	90.432	74.554	67.175	1.00 61.53	F
ATOM	8915	NZ	LYS	F	4	90.788	73.874	65.896	1.00 70.19	F
ATOM	8916	C	LYS	F	4	86.127	72.577	65.958	1.00 39.28	F
ATOM	8917	O	LYS	F	4	85.294	72.817	66.831	1.00 39.09	F
ATOM	8918	N	THR	F	5	86.764	71.427	65.854	1.00 40.82	F
ATOM	8919	CA	THR	F	5	86.507	70.316	66.717	1.00 36.59	F
ATOM	8920	CB	THR	F	5	86.375	69.051	65.844	1.00 34.26	F
ATOM	8921	OG1	THR	F	5	85.177	68.363	66.198	1.00 41.95	F
ATOM	8922	CG2	THR	F	5	87.547	68.157	65.979	1.00 26.04	F
ATOM	8923	C	THR	F	5	87.627	70.240	67.730	1.00 35.59	F
ATOM	8924	O	THR	F	5	88.792	70.435	67.401	1.00 38.72	F
ATOM	8925	N	ALA	F	6	87.254	69.996	68.979	1.00 36.62	F
ATOM	8926	CA	ALA	F	6	88.208	69.912	70.076	1.00 34.75	F
ATOM	8927	CB	ALA	F	6	87.492	69.541	71.354	1.00 32.49	F
ATOM	8928	C	ALA	F	6	89.282	68.902	69.773	1.00 36.90	F
ATOM	8929	O	ALA	F	6	90.390	68.975	70.291	1.00 37.23	F
ATOM	8930	N	ASN	F	7	88.948	67.953	68.916	1.00 45.57	F
ATOM	8931	CA	ASN	F	7	89.887	66.904	68.537	1.00 49.55	F
ATOM	8932	CB	ASN	F	7	89.151	65.768	67.845	1.00 51.09	F
ATOM	8933	CG	ASN	F	7	89.688	64.422	68.235	1.00 57.54	F
ATOM	8934	OD1	ASN	F	7	90.699	64.329	68.943	1.00 59.53	F
ATOM	8935	ND2	ASN	F	7	89.019	63.362	67.783	1.00 49.46	F
ATOM	8936	C	ASN	F	7	90.940	67.449	67.608	1.00 48.81	F
ATOM	8937	O	ASN	F	7	92.106	67.046	67.666	1.00 53.22	F
ATOM	8938	N	GLY	F	8	90.508	68.363	66.750	1.00 47.63	F
ATOM	8939	CA	GLY	F	8	91.406	68.988	65.806	1.00 53.31	F
ATOM	8940	C	GLY	F	8	90.738	69.585	64.568	1.00 57.85	F
ATOM	8941	O	GLY	F	8	90.991	70.750	64.226	1.00 59.56	F



ATOM	8942	N	THR	F	9	89.876	68.801	63.910	1.00	53.29	F
ATOM	8943	CA	THR	F	9	89.202	69.206	62.672	1.00	49.01	F
ATOM	8944	CB	THR	F	9	88.340	68.067	62.160	1.00	51.01	F
ATOM	8945	OG1	THR	F	9	89.162	66.901	62.022	1.00	63.11	F
ATOM	8946	CG2	THR	F	9	87.738	68.415	60.810	1.00	47.64	F
ATOM	8947	C	THR	F	9	88.379	70.489	62.629	1.00	47.40	F
ATOM	8948	O	THR	F	9	87.712	70.854	63.588	1.00	49.35	F
ATOM	8949	N	ALA	F	10	88.423	71.154	61.474	1.00	44.85	F
ATOM	8950	CA	ALA	F	10	87.717	72.415	61.249	1.00	38.12	F
ATOM	8951	CB	ALA	F	10	88.721	73.552	61.113	1.00	27.66	F
ATOM	8952	C	ALA	F	10	86.840	72.408	60.017	1.00	36.08	F
ATOM	8953	O	ALA	F	10	87.027	71.606	59.105	1.00	39.20	F
ATOM	8954	N	ILE	F	11	85.869	73.311	60.008	1.00	31.43	F
ATOM	8955	CA	ILE	F	11	85.001	73.485	58.860	1.00	32.87	F
ATOM	8956	CB	ILE	F	11	83.554	73.186	59.172	1.00	34.87	F
ATOM	8957	CG2	ILE	F	11	82.728	73.391	57.916	1.00	35.36	F
ATOM	8958	CG1	ILE	F	11	83.421	71.755	59.699	1.00	37.73	F
ATOM	8959	CD1	ILE	F	11	82.010	71.357	60.058	1.00	34.84	F
ATOM	8960	C	ILE	F	11	85.160	74.965	58.625	1.00	33.05	F
ATOM	8961	O	ILE	F	11	84.819	75.771	59.476	1.00	40.18	F
ATOM	8962	N	PRO	F	12	85.680	75.347	57.468	1.00	29.45	F
ATOM	8963	CD	PRO	F	12	86.123	74.482	56.362	1.00	31.75	F
ATOM	8964	CA	PRO	F	12	85.898	76.753	57.147	1.00	31.33	F
ATOM	8965	CB	PRO	F	12	86.914	76.670	56.018	1.00	35.39	F
ATOM	8966	CG	PRO	F	12	86.406	75.486	55.244	1.00	32.23	F
ATOM	8967	C	PRO	F	12	84.696	77.592	56.752	1.00	32.57	F
ATOM	8968	O	PRO	F	12	83.570	77.093	56.661	1.00	31.88	F
ATOM	8969	N	ILE	F	13	84.983	78.878	56.520	1.00	31.86	F
ATOM	8970	CA	ILE	F	13	84.017	79.885	56.073	1.00	31.16	F
ATOM	8971	CB	ILE	F	13	84.750	81.185	55.638	1.00	32.37	F
ATOM	8972	CG2	ILE	F	13	83.809	82.104	54.849	1.00	31.26	F
ATOM	8973	CG1	ILE	F	13	85.328	81.882	56.873	1.00	32.40	F
ATOM	8974	CD1	ILE	F	13	86.079	83.116	56.569	1.00	26.26	F
ATOM	8975	C	ILE	F	13	83.304	79.310	54.864	1.00	29.77	F
ATOM	8976	O	ILE	F	13	83.961	78.796	53.969	1.00	31.36	F
ATOM	8977	N	GLY	F	14	81.976	79.387	54.838	1.00	27.74	F
ATOM	8978	CA	GLY	F	14	81.228	78.849	53.714	1.00	28.67	F
ATOM	8979	C	GLY	F	14	80.606	77.490	54.011	1.00	33.28	F
ATOM	8980	O	GLY	F	14	79.811	76.961	53.223	1.00	34.40	F
ATOM	8981	N	GLY	F	15	80.982	76.902	55.141	1.00	33.08	F
ATOM	8982	CA	GLY	F	15	80.407	75.622	55.517	1.00	30.57	F
ATOM	8983	C	GLY	F	15	81.160	74.389	55.063	1.00	31.84	F
ATOM	8984	O	GLY	F	15	82.195	74.473	54.401	1.00	34.18	F
ATOM	8985	N	GLY	F	16	80.614	73.232	55.422	1.00	27.95	F
ATOM	8986	CA	GLY	F	16	81.226	71.966	55.087	1.00	20.25	F
ATOM	8987	C	GLY	F	16	80.855	70.962	56.155	1.00	20.58	F
ATOM	8988	O	GLY	F	16	79.848	71.114	56.836	1.00	26.27	F
ATOM	8989	N	SER	F	17	81.666	69.941	56.354	1.00	17.51	F
ATOM	8990	CA	SER	F	17	81.298	68.954	57.343	1.00	16.79	F
ATOM	8991	CB	SER	F	17	80.490	67.847	56.665	1.00	22.29	F
ATOM	8992	OG	SER	F	17	81.331	66.996	55.896	1.00	27.14	F
ATOM	8993	C	SER	F	17	82.473	68.343	58.060	1.00	15.13	F
ATOM	8994	O	SER	F	17	83.583	68.326	57.541	1.00	18.53	F
ATOM	8995	N	ALA	F	18	82.230	67.822	59.257	1.00	13.27	F
ATOM	8996	CA	ALA	F	18	83.302	67.191	60.020	1.00	15.38	F
ATOM	8997	CB	ALA	F	18	84.042	68.213	60.837	1.00	10.31	F
ATOM	8998	C	ALA	F	18	82.787	66.119	60.930	1.00	21.83	F
ATOM	8999	O	ALA	F	18	81.616	66.105	61.300	1.00	31.45	F



ATOM	9000	N	ASN	F	19	83.685	65.222	61.301	1.00	22.39	F
ATOM	9001	CA	ASN	F	19	83.368	64.129	62.202	1.00	21.13	F
ATOM	9002	CB	ASN	F	19	84.265	62.916	61.930	1.00	19.51	F
ATOM	9003	CG	ASN	F	19	83.837	62.124	60.708	1.00	19.53	F
ATOM	9004	OD1	ASN	F	19	82.875	62.470	60.029	1.00	15.43	F
ATOM	9005	ND2	ASN	F	19	84.564	61.052	60.421	1.00	13.23	F
ATOM	9006	C	ASN	F	19	83.636	64.572	63.621	1.00	24.69	F
ATOM	9007	O	ASN	F	19	84.599	65.278	63.889	1.00	26.24	F
ATOM	9008	N	VAL	F	20	82.792	64.145	64.541	1.00	27.12	F
ATOM	9009	CA	VAL	F	20	83.017	64.459	65.936	1.00	27.32	F
ATOM	9010	CB	VAL	F	20	81.945	65.391	66.451	1.00	28.40	F
ATOM	9011	CG1	VAL	F	20	82.293	65.810	67.861	1.00	30.24	F
ATOM	9012	CG2	VAL	F	20	81.849	66.602	65.528	1.00	18.25	F
ATOM	9013	C	VAL	F	20	82.999	63.129	66.690	1.00	25.96	F
ATOM	9014	O	VAL	F	20	81.965	62.473	66.774	1.00	28.82	F
ATOM	9015	N	TYR	F	21	84.151	62.726	67.213	1.00	23.34	F
ATOM	9016	CA	TYR	F	21	84.279	61.454	67.940	1.00	26.68	F
ATOM	9017	CB	TYR	F	21	85.650	60.844	67.653	1.00	19.01	F
ATOM	9018	CG	TYR	F	21	85.959	60.791	66.182	1.00	28.25	F
ATOM	9019	CD1	TYR	F	21	86.786	61.740	65.592	1.00	24.71	F
ATOM	9020	CE1	TYR	F	21	87.030	61.723	64.214	1.00	31.01	F
ATOM	9021	CD2	TYR	F	21	85.379	59.814	65.359	1.00	25.81	F
ATOM	9022	CE2	TYR	F	21	85.618	59.787	63.988	1.00	29.45	F
ATOM	9023	CZ	TYR	F	21	86.447	60.744	63.422	1.00	34.73	F
ATOM	9024	OH	TYR	F	21	86.723	60.710	62.078	1.00	35.46	F
ATOM	9025	C	TYR	F	21	84.069	61.562	69.455	1.00	29.69	F
ATOM	9026	O	TYR	F	21	84.840	62.230	70.155	1.00	33.08	F
ATOM	9027	N	VAL	F	22	83.048	60.869	69.963	1.00	31.10	F
ATOM	9028	CA	VAL	F	22	82.704	60.925	71.390	1.00	30.65	F
ATOM	9029	CB	VAL	F	22	81.277	61.440	71.602	1.00	25.94	F
ATOM	9030	CG1	VAL	F	22	81.109	62.803	70.978	1.00	23.02	F
ATOM	9031	CG2	VAL	F	22	80.299	60.455	71.013	1.00	24.67	F
ATOM	9032	C	VAL	F	22	82.772	59.646	72.202	1.00	31.76	F
ATOM	9033	O	VAL	F	22	82.265	58.607	71.773	1.00	30.44	F
ATOM	9034	N	ASN	F	23	83.371	59.740	73.391	1.00	32.82	F
ATOM	9035	CA	ASN	F	23	83.441	58.607	74.308	1.00	32.03	F
ATOM	9036	CB	ASN	F	23	84.661	58.721	75.179	1.00	32.85	F
ATOM	9037	CG	ASN	F	23	85.867	59.131	74.410	1.00	34.07	F
ATOM	9038	OD1	ASN	F	23	86.613	58.303	73.879	1.00	34.83	F
ATOM	9039	ND2	ASN	F	23	86.068	60.431	74.326	1.00	43.60	F
ATOM	9040	C	ASN	F	23	82.195	58.748	75.183	1.00	31.34	F
ATOM	9041	O	ASN	F	23	82.003	59.786	75.803	1.00	29.30	F
ATOM	9042	N	LEU	F	24	81.353	57.721	75.222	1.00	31.60	F
ATOM	9043	CA	LEU	F	24	80.114	57.766	76.009	1.00	32.96	F
ATOM	9044	CB	LEU	F	24	78.938	57.325	75.129	1.00	29.44	F
ATOM	9045	CG	LEU	F	24	78.785	57.994	73.764	1.00	25.79	F
ATOM	9046	CD1	LEU	F	24	78.076	57.049	72.820	1.00	22.87	F
ATOM	9047	CD2	LEU	F	24	78.018	59.293	73.886	1.00	28.59	F
ATOM	9048	C	LEU	F	24	80.143	56.869	77.256	1.00	33.03	F
ATOM	9049	O	LEU	F	24	80.927	55.925	77.324	1.00	36.91	F
ATOM	9050	N	ALA	F	25	79.290	57.166	78.236	1.00	29.98	F
ATOM	9051	CA	ALA	F	25	79.184	56.338	79.446	1.00	29.57	F
ATOM	9052	CB	ALA	F	25	77.962	56.726	80.201	1.00	25.78	F
ATOM	9053	C	ALA	F	25	79.051	54.891	78.974	1.00	32.98	F
ATOM	9054	O	ALA	F	25	78.171	54.573	78.192	1.00	39.53	F
ATOM	9055	N	PRO	F	26	79.900	53.992	79.455	1.00	31.64	F
ATOM	9056	CD	PRO	F	26	80.913	54.190	80.491	1.00	34.85	F
ATOM	9057	CA	PRO	F	26	79.856	52.584	79.039	1.00	33.70	F



ATOM	9058	CB	PRO	F	26	81.065	51.963	79.765	1.00	35.76	F
ATOM	9059	CG	PRO	F	26	81.916	53.110	80.123	1.00	41.95	F
ATOM	9060	C	PRO	F	26	78.570	51.802	79.343	1.00	35.04	F
ATOM	9061	O	PRO	F	26	78.246	50.830	78.654	1.00	30.95	F
ATOM	9062	N	VAL	F	27	77.862	52.226	80.386	1.00	35.37	F
ATOM	9063	CA	VAL	F	27	76.642	51.575	80.840	1.00	31.59	F
ATOM	9064	CB	VAL	F	27	76.906	50.790	82.128	1.00	34.64	F
ATOM	9065	CG1	VAL	F	27	75.607	50.240	82.691	1.00	35.51	F
ATOM	9066	CG2	VAL	F	27	77.907	49.697	81.865	1.00	33.14	F
ATOM	9067	C	VAL	F	27	75.562	52.583	81.161	1.00	31.10	F
ATOM	9068	O	VAL	F	27	75.809	53.593	81.802	1.00	34.90	F
ATOM	9069	N	VAL	F	28	74.348	52.290	80.745	1.00	32.54	F
ATOM	9070	CA	VAL	F	28	73.227	53.177	81.012	1.00	34.96	F
ATOM	9071	CB	VAL	F	28	72.965	54.118	79.808	1.00	31.97	F
ATOM	9072	CG1	VAL	F	28	71.854	55.105	80.119	1.00	34.44	F
ATOM	9073	CG2	VAL	F	28	74.230	54.851	79.459	1.00	30.03	F
ATOM	9074	C	VAL	F	28	72.036	52.248	81.234	1.00	40.51	F
ATOM	9075	O	VAL	F	28	71.858	51.255	80.513	1.00	42.64	F
ATOM	9076	N	ASN	F	29	71.226	52.553	82.240	1.00	41.21	F
ATOM	9077	CA	ASN	F	29	70.081	51.705	82.538	1.00	40.01	F
ATOM	9078	CB	ASN	F	29	69.848	51.600	84.043	1.00	33.89	F
ATOM	9079	CG	ASN	F	29	71.058	51.096	84.780	1.00	39.67	F
ATOM	9080	OD1	ASN	F	29	71.560	50.014	84.496	1.00	43.68	F
ATOM	9081	ND2	ASN	F	29	71.539	51.879	85.743	1.00	47.58	F
ATOM	9082	C	ASN	F	29	68.831	52.244	81.924	1.00	38.61	F
ATOM	9083	O	ASN	F	29	68.730	53.443	81.643	1.00	34.33	F
ATOM	9084	N	VAL	F	30	67.867	51.350	81.736	1.00	36.25	F
ATOM	9085	CA	VAL	F	30	66.590	51.758	81.199	1.00	38.11	F
ATOM	9086	CB	VAL	F	30	65.587	50.599	81.221	1.00	36.54	F
ATOM	9087	CG1	VAL	F	30	64.214	51.075	80.744	1.00	31.95	F
ATOM	9088	CG2	VAL	F	30	66.094	49.466	80.337	1.00	31.08	F
ATOM	9089	C	VAL	F	30	66.147	52.841	82.166	1.00	41.13	F
ATOM	9090	O	VAL	F	30	66.435	52.751	83.355	1.00	42.21	F
ATOM	9091	N	GLY	F	31	65.497	53.882	81.661	1.00	45.46	F
ATOM	9092	CA	GLY	F	31	65.038	54.941	82.542	1.00	50.57	F
ATOM	9093	C	GLY	F	31	66.019	56.082	82.739	1.00	54.66	F
ATOM	9094	O	GLY	F	31	65.601	57.218	82.947	1.00	57.31	F
ATOM	9095	N	GLN	F	32	67.317	55.795	82.674	1.00	54.51	F
ATOM	9096	CA	GLN	F	32	68.337	56.826	82.845	1.00	53.70	F
ATOM	9097	CB	GLN	F	32	69.630	56.188	83.342	1.00	54.96	F
ATOM	9098	CG	GLN	F	32	69.729	56.091	84.847	1.00	66.08	F
ATOM	9099	CD	GLN	F	32	70.815	55.124	85.296	1.00	73.26	F
ATOM	9100	OE1	GLN	F	32	71.911	55.085	84.720	1.00	71.06	F
ATOM	9101	NE2	GLN	F	32	70.518	54.339	86.340	1.00	75.66	F
ATOM	9102	C	GLN	F	32	68.627	57.656	81.583	1.00	53.14	F
ATOM	9103	O	GLN	F	32	68.056	57.430	80.516	1.00	51.96	F
ATOM	9104	N	ASN	F	33	69.518	58.630	81.729	1.00	51.12	F
ATOM	9105	CA	ASN	F	33	69.908	59.502	80.630	1.00	47.87	F
ATOM	9106	CB	ASN	F	33	69.747	60.968	81.024	1.00	42.01	F
ATOM	9107	CG	ASN	F	33	68.438	61.561	80.553	1.00	45.78	F
ATOM	9108	OD1	ASN	F	33	68.066	62.669	80.951	1.00	38.33	F
ATOM	9109	ND2	ASN	F	33	67.735	60.837	79.689	1.00	43.12	F
ATOM	9110	C	ASN	F	33	71.347	59.299	80.187	1.00	48.45	F
ATOM	9111	O	ASN	F	33	72.271	59.220	80.996	1.00	48.59	F
ATOM	9112	N	LEU	F	34	71.527	59.186	78.885	1.00	50.50	F
ATOM	9113	CA	LEU	F	34	72.856	59.079	78.314	1.00	48.19	F
ATOM	9114	CB	LEU	F	34	72.873	58.110	77.142	1.00	48.47	F
ATOM	9115	CG	LEU	F	34	74.152	58.169	76.321	1.00	45.89	F



ATOM	9116	CD1	LEU	F	34	75.297	57.484	77.046	1.00	42.48	F
ATOM	9117	CD2	LEU	F	34	73.874	57.510	74.990	1.00	49.15	F
ATOM	9118	C	LEU	F	34	73.013	60.509	77.812	1.00	47.21	F
ATOM	9119	O	LEU	F	34	72.134	61.041	77.113	1.00	43.62	F
ATOM	9120	N	VAL	F	35	74.108	61.150	78.183	1.00	43.20	F
ATOM	9121	CA	VAL	F	35	74.284	62.519	77.764	1.00	41.46	F
ATOM	9122	CB	VAL	F	35	74.430	63.441	78.984	1.00	41.50	F
ATOM	9123	CG1	VAL	F	35	74.542	64.883	78.538	1.00	38.83	F
ATOM	9124	CG2	VAL	F	35	73.232	63.260	79.892	1.00	37.25	F
ATOM	9125	C	VAL	F	35	75.467	62.712	76.851	1.00	37.06	F
ATOM	9126	O	VAL	F	35	76.590	62.344	77.194	1.00	37.06	F
ATOM	9127	N	VAL	F	36	75.201	63.277	75.677	1.00	34.47	F
ATOM	9128	CA	VAL	F	36	76.265	63.553	74.725	1.00	36.32	F
ATOM	9129	CB	VAL	F	36	75.959	63.024	73.328	1.00	38.02	F
ATOM	9130	CG1	VAL	F	36	77.263	62.774	72.612	1.00	41.12	F
ATOM	9131	CG2	VAL	F	36	75.146	61.757	73.409	1.00	37.10	F
ATOM	9132	C	VAL	F	36	76.336	65.047	74.654	1.00	34.58	F
ATOM	9133	O	VAL	F	36	75.472	65.691	74.054	1.00	34.73	F
ATOM	9134	N	ASP	F	37	77.356	65.610	75.284	1.00	36.96	F
ATOM	9135	CA	ASP	F	37	77.495	67.061	75.296	1.00	43.47	F
ATOM	9136	CB	ASP	F	37	77.906	67.525	76.693	1.00	46.50	F
ATOM	9137	CG	ASP	F	37	77.849	69.028	76.845	1.00	55.92	F
ATOM	9138	OD1	ASP	F	37	76.826	69.633	76.431	1.00	59.16	F
ATOM	9139	OD2	ASP	F	37	78.826	69.599	77.386	1.00	58.57	F
ATOM	9140	C	ASP	F	37	78.498	67.544	74.258	1.00	40.22	F
ATOM	9141	O	ASP	F	37	79.708	67.411	74.442	1.00	41.05	F
ATOM	9142	N	LEU	F	38	77.992	68.118	73.175	1.00	37.20	F
ATOM	9143	CA	LEU	F	38	78.870	68.579	72.112	1.00	39.70	F
ATOM	9144	CB	LEU	F	38	78.125	68.526	70.783	1.00	36.96	F
ATOM	9145	CG	LEU	F	38	77.812	67.057	70.508	1.00	30.31	F
ATOM	9146	CD1	LEU	F	38	76.853	66.949	69.386	1.00	44.81	F
ATOM	9147	CD2	LEU	F	38	79.077	66.305	70.179	1.00	34.21	F
ATOM	9148	C	LEU	F	38	79.490	69.945	72.340	1.00	39.97	F
ATOM	9149	O	LEU	F	38	80.518	70.271	71.726	1.00	34.44	F
ATOM	9150	N	SER	F	39	78.868	70.719	73.234	1.00	42.07	F
ATOM	9151	CA	SER	F	39	79.330	72.059	73.608	1.00	39.92	F
ATOM	9152	CB	SER	F	39	78.472	72.639	74.725	1.00	43.81	F
ATOM	9153	OG	SER	F	39	78.915	72.141	75.981	1.00	39.88	F
ATOM	9154	C	SER	F	39	80.730	71.893	74.158	1.00	35.42	F
ATOM	9155	O	SER	F	39	81.441	72.853	74.403	1.00	38.86	F
ATOM	9156	N	THR	F	40	81.114	70.656	74.381	1.00	31.46	F
ATOM	9157	CA	THR	F	40	82.429	70.398	74.890	1.00	30.14	F
ATOM	9158	CB	THR	F	40	82.368	69.253	75.910	1.00	28.16	F
ATOM	9159	OG1	THR	F	40	82.804	69.753	77.172	1.00	36.75	F
ATOM	9160	CG2	THR	F	40	83.241	68.079	75.503	1.00	23.29	F
ATOM	9161	C	THR	F	40	83.350	70.042	73.739	1.00	31.05	F
ATOM	9162	O	THR	F	40	84.572	70.011	73.892	1.00	28.36	F
ATOM	9163	N	GLN	F	41	82.765	69.789	72.571	1.00	33.63	F
ATOM	9164	CA	GLN	F	41	83.573	69.382	71.432	1.00	36.47	F
ATOM	9165	CB	GLN	F	41	83.286	67.922	71.121	1.00	40.54	F
ATOM	9166	CG	GLN	F	41	83.720	66.995	72.226	1.00	40.60	F
ATOM	9167	CD	GLN	F	41	84.377	65.774	71.673	1.00	48.50	F
ATOM	9168	OE1	GLN	F	41	83.710	64.857	71.182	1.00	50.59	F
ATOM	9169	NE2	GLN	F	41	85.704	65.754	71.714	1.00	55.45	F
ATOM	9170	C	GLN	F	41	83.460	70.193	70.152	1.00	36.38	F
ATOM	9171	O	GLN	F	41	84.242	69.984	69.223	1.00	32.40	F
ATOM	9172	N	ILE	F	42	82.499	71.112	70.098	1.00	34.19	F
ATOM	9173	CA	ILE	F	42	82.320	71.928	68.908	1.00	33.92	F



ATOM	9174	CB	ILE	F	42	81.025	71.550	68.200	1.00	29.76	F
ATOM	9175	CG2	ILE	F	42	80.872	72.358	66.935	1.00	33.58	F
ATOM	9176	CG1	ILE	F	42	81.040	70.062	67.872	1.00	31.94	F
ATOM	9177	CD1	ILE	F	42	79.741	69.572	67.315	1.00	32.41	F
ATOM	9178	C	ILE	F	42	82.316	73.425	69.224	1.00	37.57	F
ATOM	9179	O	ILE	F	42	81.462	73.920	69.981	1.00	34.58	F
ATOM	9180	N	PHE	F	43	83.276	74.133	68.625	1.00	40.15	F
ATOM	9181	CA	PHE	F	43	83.439	75.571	68.823	1.00	39.76	F
ATOM	9182	CB	PHE	F	43	84.757	75.846	69.528	1.00	37.57	F
ATOM	9183	CG	PHE	F	43	84.880	75.158	70.836	1.00	38.48	F
ATOM	9184	CD1	PHE	F	43	85.320	73.841	70.900	1.00	39.96	F
ATOM	9185	CD2	PHE	F	43	84.491	75.803	72.013	1.00	41.38	F
ATOM	9186	CE1	PHE	F	43	85.373	73.164	72.123	1.00	40.49	F
ATOM	9187	CE2	PHE	F	43	84.538	75.142	73.242	1.00	40.63	F
ATOM	9188	CZ	PHE	F	43	84.979	73.818	73.300	1.00	35.43	F
ATOM	9189	C	PHE	F	43	83.394	76.404	67.561	1.00	39.77	F
ATOM	9190	O	PHE	F	43	83.897	76.000	66.520	1.00	42.10	F
ATOM	9191	N	CYS	F	44	82.796	77.581	67.667	1.00	39.38	F
ATOM	9192	CA	CYS	F	44	82.724	78.492	66.535	1.00	39.84	F
ATOM	9193	C	CYS	F	44	83.115	79.913	66.973	1.00	40.53	F
ATOM	9194	O	CYS	F	44	83.271	80.200	68.163	1.00	41.58	F
ATOM	9195	CB	CYS	F	44	81.318	78.491	65.961	1.00	43.15	F
ATOM	9196	SG	CYS	F	44	80.664	76.852	65.512	1.00	47.68	F
ATOM	9197	N	HIS	F	45	83.292	80.801	66.005	1.00	38.76	F
ATOM	9198	CA	HIS	F	45	83.667	82.172	66.305	1.00	35.21	F
ATOM	9199	CB	HIS	F	45	85.179	82.311	66.496	1.00	30.76	F
ATOM	9200	CG	HIS	F	45	85.963	82.118	65.237	1.00	37.14	F
ATOM	9201	CD2	HIS	F	45	86.027	82.859	64.105	1.00	40.88	F
ATOM	9202	ND1	HIS	F	45	86.758	81.016	65.016	1.00	38.71	F
ATOM	9203	CE1	HIS	F	45	87.274	81.083	63.801	1.00	39.21	F
ATOM	9204	NE2	HIS	F	45	86.846	82.192	63.226	1.00	37.14	F
ATOM	9205	C	HIS	F	45	83.251	83.016	65.135	1.00	36.46	F
ATOM	9206	O	HIS	F	45	83.095	82.506	64.027	1.00	39.68	F
ATOM	9207	N	ASN	F	46	83.070	84.304	65.401	1.00	39.38	F
ATOM	9208	CA	ASN	F	46	82.689	85.303	64.409	1.00	39.94	F
ATOM	9209	CB	ASN	F	46	81.971	86.445	65.126	1.00	43.78	F
ATOM	9210	CG	ASN	F	46	81.235	87.358	64.183	1.00	44.11	F
ATOM	9211	OD1	ASN	F	46	81.747	87.726	63.125	1.00	45.58	F
ATOM	9212	ND2	ASN	F	46	80.027	87.742	64.567	1.00	37.43	F
ATOM	9213	C	ASN	F	46	84.023	85.794	63.839	1.00	41.13	F
ATOM	9214	O	ASN	F	46	84.981	85.959	64.586	1.00	38.92	F
ATOM	9215	N	ASP	F	47	84.111	86.020	62.534	1.00	44.83	F
ATOM	9216	CA	ASP	F	47	85.384	86.477	61.974	1.00	48.14	F
ATOM	9217	CB	ASP	F	47	85.613	85.867	60.582	1.00	46.39	F
ATOM	9218	CG	ASP	F	47	86.111	84.423	60.644	1.00	44.27	F
ATOM	9219	OD1	ASP	F	47	87.125	84.179	61.330	1.00	47.40	F
ATOM	9220	OD2	ASP	F	47	85.501	83.534	60.007	1.00	41.51	F
ATOM	9221	C	ASP	F	47	85.496	88.006	61.916	1.00	49.87	F
ATOM	9222	O	ASP	F	47	86.595	88.565	61.931	1.00	49.10	F
ATOM	9223	N	TYR	F	48	84.355	88.682	61.860	1.00	51.31	F
ATOM	9224	CA	TYR	F	48	84.346	90.134	61.821	1.00	52.11	F
ATOM	9225	CB	TYR	F	48	84.100	90.627	60.396	1.00	55.53	F
ATOM	9226	CG	TYR	F	48	85.066	90.035	59.384	1.00	64.22	F
ATOM	9227	CD1	TYR	F	48	84.737	88.873	58.672	1.00	67.04	F
ATOM	9228	CE1	TYR	F	48	85.632	88.296	57.773	1.00	68.66	F
ATOM	9229	CD2	TYR	F	48	86.323	90.608	59.166	1.00	64.64	F
ATOM	9230	CE2	TYR	F	48	87.230	90.034	58.269	1.00	68.28	F
ATOM	9231	CZ	TYR	F	48	86.874	88.876	57.581	1.00	68.66	F



ATOM	9232	OH	TYR	F	48	87.760	88.267	56.728	1.00	68.74	F
ATOM	9233	C	TYR	F	48	83.262	90.633	62.762	1.00	51.91	F
ATOM	9234	O	TYR	F	48	82.256	91.214	62.328	1.00	54.25	F
ATOM	9235	N	PRO	F	49	83.463	90.414	64.074	1.00	48.98	F
ATOM	9236	CD	PRO	F	49	84.675	89.810	64.653	1.00	50.70	F
ATOM	9237	CA	PRO	F	49	82.535	90.813	65.133	1.00	50.04	F
ATOM	9238	CB	PRO	F	49	83.290	90.453	66.413	1.00	48.62	F
ATOM	9239	CG	PRO	F	49	84.717	90.435	66.007	1.00	48.81	F
ATOM	9240	C	PRO	F	49	82.080	92.269	65.102	1.00	53.96	F
ATOM	9241	O	PRO	F	49	80.881	92.537	65.007	1.00	54.22	F
ATOM	9242	N	GLU	F	50	83.036	93.199	65.159	1.00	55.66	F
ATOM	9243	CA	GLU	F	50	82.749	94.643	65.158	1.00	53.61	F
ATOM	9244	CB	GLU	F	50	84.038	95.454	65.023	1.00	46.52	F
ATOM	9245	CG	GLU	F	50	85.145	95.079	65.977	1.00	55.75	F
ATOM	9246	CD	GLU	F	50	85.831	93.777	65.600	1.00	63.20	F
ATOM	9247	OE1	GLU	F	50	85.654	93.309	64.447	1.00	64.70	F
ATOM	9248	OE2	GLU	F	50	86.564	93.226	66.454	1.00	64.13	F
ATOM	9249	C	GLU	F	50	81.765	95.179	64.109	1.00	52.68	F
ATOM	9250	O	GLU	F	50	81.199	96.250	64.297	1.00	55.19	F
ATOM	9251	N	THR	F	51	81.549	94.464	63.013	1.00	49.84	F
ATOM	9252	CA	THR	F	51	80.646	94.977	61.988	1.00	53.47	F
ATOM	9253	CB	THR	F	51	81.454	95.486	60.761	1.00	53.02	F
ATOM	9254	OG1	THR	F	51	81.741	94.406	59.858	1.00	49.48	F
ATOM	9255	CG2	THR	F	51	82.774	96.054	61.234	1.00	54.99	F
ATOM	9256	C	THR	F	51	79.631	93.934	61.532	1.00	57.58	F
ATOM	9257	O	THR	F	51	78.664	94.247	60.823	1.00	57.30	F
ATOM	9258	N	ILE	F	52	79.850	92.686	61.935	1.00	55.85	F
ATOM	9259	CA	ILE	F	52	78.934	91.636	61.545	1.00	50.11	F
ATOM	9260	CB	ILE	F	52	79.563	90.725	60.494	1.00	50.95	F
ATOM	9261	CG2	ILE	F	52	78.594	89.599	60.131	1.00	50.05	F
ATOM	9262	CG1	ILE	F	52	79.911	91.547	59.250	1.00	49.40	F
ATOM	9263	CD1	ILE	F	52	80.579	90.746	58.162	1.00	47.71	F
ATOM	9264	C	ILE	F	52	78.510	90.803	62.725	1.00	47.97	F
ATOM	9265	O	ILE	F	52	79.320	90.465	63.578	1.00	46.12	F
ATOM	9266	N	THR	F	53	77.219	90.502	62.787	1.00	47.89	F
ATOM	9267	CA	THR	F	53	76.688	89.672	63.855	1.00	50.10	F
ATOM	9268	CB	THR	F	53	75.505	90.354	64.578	1.00	52.79	F
ATOM	9269	OG1	THR	F	53	76.011	91.280	65.552	1.00	48.04	F
ATOM	9270	CG2	THR	F	53	74.629	89.314	65.276	1.00	49.03	F
ATOM	9271	C	THR	F	53	76.236	88.352	63.249	1.00	49.60	F
ATOM	9272	O	THR	F	53	75.434	88.329	62.306	1.00	49.63	F
ATOM	9273	N	ASP	F	54	76.765	87.257	63.791	1.00	49.87	F
ATOM	9274	CA	ASP	F	54	76.441	85.918	63.301	1.00	50.24	F
ATOM	9275	CB	ASP	F	54	77.706	85.035	63.298	1.00	48.39	F
ATOM	9276	CG	ASP	F	54	78.693	85.416	62.192	1.00	45.32	F
ATOM	9277	OD1	ASP	F	54	78.243	85.670	61.055	1.00	45.90	F
ATOM	9278	OD2	ASP	F	54	79.918	85.447	62.452	1.00	44.36	F
ATOM	9279	C	ASP	F	54	75.327	85.223	64.094	1.00	48.69	F
ATOM	9280	O	ASP	F	54	75.265	85.320	65.324	1.00	45.65	F
ATOM	9281	N	TYR	F	55	74.461	84.519	63.363	1.00	50.52	F
ATOM	9282	CA	TYR	F	55	73.331	83.767	63.928	1.00	50.37	F
ATOM	9283	CB	TYR	F	55	72.029	84.208	63.274	1.00	50.69	F
ATOM	9284	CG	TYR	F	55	71.762	85.687	63.366	1.00	54.96	F
ATOM	9285	CD1	TYR	F	55	71.346	86.399	62.236	1.00	53.99	F
ATOM	9286	CE1	TYR	F	55	71.107	87.761	62.291	1.00	57.00	F
ATOM	9287	CD2	TYR	F	55	71.929	86.381	64.571	1.00	52.15	F
ATOM	9288	CE2	TYR	F	55	71.687	87.754	64.643	1.00	59.82	F
ATOM	9289	CZ	TYR	F	55	71.278	88.440	63.491	1.00	59.09	F



ATOM	9290	OH	TYR	F	55	71.054	89.800	63.521	1.00	53.63	F
ATOM	9291	C	TYR	F	55	73.486	82.263	63.704	1.00	46.89	F
ATOM	9292	O	TYR	F	55	73.431	81.790	62.570	1.00	45.92	F
ATOM	9293	N	VAL	F	56	73.670	81.522	64.790	1.00	45.33	F
ATOM	9294	CA	VAL	F	56	73.828	80.078	64.714	1.00	44.46	F
ATOM	9295	CB	VAL	F	56	74.998	79.626	65.564	1.00	46.20	F
ATOM	9296	CG1	VAL	F	56	75.108	78.108	65.530	1.00	45.80	F
ATOM	9297	CG2	VAL	F	56	76.260	80.261	65.033	1.00	47.31	F
ATOM	9298	C	VAL	F	56	72.565	79.360	65.164	1.00	43.21	F
ATOM	9299	O	VAL	F	56	72.001	79.653	66.206	1.00	45.21	F
ATOM	9300	N	THR	F	57	72.154	78.376	64.387	1.00	43.55	F
ATOM	9301	CA	THR	F	57	70.917	77.659	64.656	1.00	40.66	F
ATOM	9302	CB	THR	F	57	69.886	78.152	63.631	1.00	33.53	F
ATOM	9303	OG1	THR	F	57	68.588	78.182	64.199	1.00	34.79	F
ATOM	9304	CG2	THR	F	57	69.886	77.263	62.437	1.00	21.98	F
ATOM	9305	C	THR	F	57	71.091	76.133	64.508	1.00	40.60	F
ATOM	9306	O	THR	F	57	71.965	75.688	63.767	1.00	42.05	F
ATOM	9307	N	LEU	F	58	70.283	75.337	65.215	1.00	38.61	F
ATOM	9308	CA	LEU	F	58	70.357	73.882	65.054	1.00	41.47	F
ATOM	9309	CB	LEU	F	58	70.056	73.131	66.357	1.00	39.80	F
ATOM	9310	CG	LEU	F	58	69.934	71.602	66.154	1.00	38.42	F
ATOM	9311	CD1	LEU	F	58	71.288	71.027	65.764	1.00	34.72	F
ATOM	9312	CD2	LEU	F	58	69.430	70.919	67.411	1.00	32.56	F
ATOM	9313	C	LEU	F	58	69.324	73.485	63.990	1.00	42.93	F
ATOM	9314	O	LEU	F	58	68.216	73.041	64.311	1.00	44.09	F
ATOM	9315	N	GLN	F	59	69.715	73.657	62.727	1.00	41.95	F
ATOM	9316	CA	GLN	F	59	68.889	73.369	61.556	1.00	41.80	F
ATOM	9317	CB	GLN	F	59	69.776	73.398	60.308	1.00	48.74	F
ATOM	9318	CG	GLN	F	59	69.257	74.221	59.128	1.00	59.59	F
ATOM	9319	CD	GLN	F	59	67.850	73.851	58.708	1.00	66.26	F
ATOM	9320	OE1	GLN	F	59	66.869	74.294	59.310	1.00	70.05	F
ATOM	9321	NE2	GLN	F	59	67.742	73.026	57.673	1.00	71.52	F
ATOM	9322	C	GLN	F	59	68.147	72.028	61.605	1.00	39.89	F
ATOM	9323	O	GLN	F	59	66.941	71.965	61.356	1.00	37.86	F
ATOM	9324	N	ARG	F	60	68.881	70.960	61.911	1.00	37.41	F
ATOM	9325	CA	ARG	F	60	68.315	69.616	61.974	1.00	35.64	F
ATOM	9326	CB	ARG	F	60	68.231	69.040	60.559	1.00	35.40	F
ATOM	9327	CG	ARG	F	60	67.434	67.758	60.407	1.00	43.14	F
ATOM	9328	CD	ARG	F	60	67.551	67.196	58.987	1.00	53.81	F
ATOM	9329	NE	ARG	F	60	67.924	68.223	58.007	1.00	71.63	F
ATOM	9330	CZ	ARG	F	60	67.167	69.269	57.663	1.00	78.01	F
ATOM	9331	NH1	ARG	F	60	65.967	69.450	58.212	1.00	80.35	F
ATOM	9332	NH2	ARG	F	60	67.616	70.153	56.775	1.00	77.33	F
ATOM	9333	C	ARG	F	60	69.175	68.710	62.860	1.00	36.20	F
ATOM	9334	O	ARG	F	60	70.372	68.934	63.030	1.00	42.72	F
ATOM	9335	N	GLY	F	61	68.551	67.695	63.437	1.00	33.59	F
ATOM	9336	CA	GLY	F	61	69.252	66.761	64.296	1.00	32.24	F
ATOM	9337	C	GLY	F	61	68.698	65.399	63.944	1.00	36.29	F
ATOM	9338	O	GLY	F	61	67.488	65.202	63.980	1.00	38.35	F
ATOM	9339	N	SER	F	62	69.571	64.457	63.604	1.00	35.65	F
ATOM	9340	CA	SER	F	62	69.119	63.141	63.208	1.00	33.23	F
ATOM	9341	CB	SER	F	62	69.277	62.987	61.704	1.00	35.05	F
ATOM	9342	OG	SER	F	62	68.519	63.977	61.037	1.00	38.93	F
ATOM	9343	C	SER	F	62	69.852	62.030	63.904	1.00	37.88	F
ATOM	9344	O	SER	F	62	71.057	62.132	64.153	1.00	42.83	F
ATOM	9345	N	ALA	F	63	69.118	60.951	64.185	1.00	37.19	F
ATOM	9346	CA	ALA	F	63	69.657	59.780	64.876	1.00	31.80	F
ATOM	9347	CB	ALA	F	63	68.672	59.299	65.904	1.00	33.96	F



ATOM	9348	C	ALA	F	63	69.979	58.650	63.921	1.00	28.53	F
ATOM	9349	O	ALA	F	63	69.353	58.520	62.885	1.00	28.53	F
ATOM	9350	N	TYR	F	64	70.961	57.834	64.293	1.00	27.17	F
ATOM	9351	CA	TYR	F	64	71.400	56.696	63.498	1.00	26.93	F
ATOM	9352	CB	TYR	F	64	72.629	57.072	62.654	1.00	29.13	F
ATOM	9353	CG	TYR	F	64	72.325	58.102	61.600	1.00	36.07	F
ATOM	9354	CD1	TYR	F	64	72.348	59.469	61.899	1.00	38.07	F
ATOM	9355	CE1	TYR	F	64	71.950	60.416	60.963	1.00	38.21	F
ATOM	9356	CD2	TYR	F	64	71.908	57.715	60.333	1.00	34.82	F
ATOM	9357	CE2	TYR	F	64	71.509	58.650	59.397	1.00	36.11	F
ATOM	9358	CZ	TYR	F	64	71.527	59.993	59.714	1.00	42.45	F
ATOM	9359	OH	TYR	F	64	71.095	60.910	58.785	1.00	51.02	F
ATOM	9360	C	TYR	F	64	71.740	55.480	64.358	1.00	26.37	F
ATOM	9361	O	TYR	F	64	72.020	55.598	65.554	1.00	25.90	F
ATOM	9362	N	GLY	F	65	71.728	54.312	63.725	1.00	25.24	F
ATOM	9363	CA	GLY	F	65	72.031	53.075	64.415	1.00	24.65	F
ATOM	9364	C	GLY	F	65	71.254	52.917	65.707	1.00	29.04	F
ATOM	9365	O	GLY	F	65	70.037	53.198	65.784	1.00	28.86	F
ATOM	9366	N	GLY	F	66	71.975	52.483	66.735	1.00	26.65	F
ATOM	9367	CA	GLY	F	66	71.363	52.258	68.025	1.00	29.12	F
ATOM	9368	C	GLY	F	66	70.588	53.435	68.546	1.00	30.54	F
ATOM	9369	O	GLY	F	66	69.475	53.283	69.012	1.00	34.98	F
ATOM	9370	N	VAL	F	67	71.164	54.621	68.466	1.00	31.58	F
ATOM	9371	CA	VAL	F	67	70.471	55.787	68.961	1.00	33.63	F
ATOM	9372	CB	VAL	F	67	71.183	57.064	68.543	1.00	34.48	F
ATOM	9373	CG1	VAL	F	67	70.259	58.257	68.766	1.00	32.71	F
ATOM	9374	CG2	VAL	F	67	72.483	57.225	69.349	1.00	29.37	F
ATOM	9375	C	VAL	F	67	69.050	55.848	68.448	1.00	36.24	F
ATOM	9376	O	VAL	F	67	68.128	56.210	69.173	1.00	40.82	F
ATOM	9377	N	LEU	F	68	68.889	55.466	67.194	1.00	37.51	F
ATOM	9378	CA	LEU	F	68	67.607	55.499	66.510	1.00	39.03	F
ATOM	9379	CB	LEU	F	68	67.880	55.383	65.017	1.00	37.37	F
ATOM	9380	CG	LEU	F	68	66.793	55.646	63.988	1.00	31.34	F
ATOM	9381	CD1	LEU	F	68	66.205	57.029	64.179	1.00	25.72	F
ATOM	9382	CD2	LEU	F	68	67.427	55.503	62.610	1.00	24.86	F
ATOM	9383	C	LEU	F	68	66.622	54.413	66.933	1.00	41.39	F
ATOM	9384	O	LEU	F	68	65.411	54.632	66.994	1.00	41.09	F
ATOM	9385	N	SER	F	69	67.141	53.240	67.241	1.00	41.05	F
ATOM	9386	CA	SER	F	69	66.273	52.137	67.593	1.00	40.78	F
ATOM	9387	CB	SER	F	69	66.769	50.867	66.911	1.00	39.72	F
ATOM	9388	OG	SER	F	69	68.104	50.585	67.296	1.00	34.71	F
ATOM	9389	C	SER	F	69	66.108	51.854	69.069	1.00	40.56	F
ATOM	9390	O	SER	F	69	65.105	51.273	69.462	1.00	43.11	F
ATOM	9391	N	ASN	F	70	67.074	52.268	69.883	1.00	38.69	F
ATOM	9392	CA	ASN	F	70	67.037	52.001	71.317	1.00	38.12	F
ATOM	9393	CB	ASN	F	70	68.330	51.302	71.736	1.00	37.38	F
ATOM	9394	CG	ASN	F	70	68.629	50.087	70.882	1.00	39.74	F
ATOM	9395	OD1	ASN	F	70	67.715	49.421	70.415	1.00	44.47	F
ATOM	9396	ND2	ASN	F	70	69.911	49.786	70.683	1.00	41.63	F
ATOM	9397	C	ASN	F	70	66.812	53.180	72.250	1.00	41.52	F
ATOM	9398	O	ASN	F	70	66.785	53.006	73.471	1.00	46.38	F
ATOM	9399	N	PHE	F	71	66.643	54.377	71.713	1.00	40.71	F
ATOM	9400	CA	PHE	F	71	66.479	55.512	72.599	1.00	37.28	F
ATOM	9401	CB	PHE	F	71	67.773	56.326	72.645	1.00	29.09	F
ATOM	9402	CG	PHE	F	71	68.948	55.591	73.224	1.00	23.70	F
ATOM	9403	CD1	PHE	F	71	69.636	54.644	72.471	1.00	27.84	F
ATOM	9404	CD2	PHE	F	71	69.373	55.849	74.537	1.00	16.77	F
ATOM	9405	CE1	PHE	F	71	70.750	53.953	73.031	1.00	36.93	F



ATOM	9406	CE2	PHE	F	71	70.469	55.177	75.101	1.00	19.07	F
ATOM	9407	CZ	PHE	F	71	71.162	54.230	74.357	1.00	23.05	F
ATOM	9408	C	PHE	F	71	65.352	56.445	72.216	1.00	41.57	F
ATOM	9409	O	PHE	F	71	64.819	56.398	71.097	1.00	43.17	F
ATOM	9410	N	SER	F	72	64.980	57.280	73.178	1.00	39.92	F
ATOM	9411	CA	SER	F	72	63.967	58.305	72.973	1.00	45.02	F
ATOM	9412	CB	SER	F	72	62.679	58.011	73.749	1.00	46.23	F
ATOM	9413	OG	SER	F	72	62.892	58.094	75.144	1.00	54.10	F
ATOM	9414	C	SER	F	72	64.703	59.477	73.586	1.00	45.49	F
ATOM	9415	O	SER	F	72	65.364	59.326	74.617	1.00	45.76	F
ATOM	9416	N	GLY	F	73	64.641	60.641	72.969	1.00	45.34	F
ATOM	9417	CA	GLY	F	73	65.398	61.705	73.576	1.00	46.34	F
ATOM	9418	C	GLY	F	73	65.116	63.112	73.159	1.00	44.44	F
ATOM	9419	O	GLY	F	73	64.289	63.387	72.279	1.00	42.38	F
ATOM	9420	N	THR	F	74	65.820	64.013	73.826	1.00	42.62	F
ATOM	9421	CA	THR	F	74	65.664	65.416	73.535	1.00	46.94	F
ATOM	9422	CB	THR	F	74	65.047	66.199	74.745	1.00	45.06	F
ATOM	9423	OG1	THR	F	74	65.981	66.231	75.829	1.00	49.66	F
ATOM	9424	CG2	THR	F	74	63.755	65.553	75.208	1.00	35.87	F
ATOM	9425	C	THR	F	74	67.013	66.020	73.200	1.00	44.87	F
ATOM	9426	O	THR	F	74	68.071	65.411	73.431	1.00	38.63	F
ATOM	9427	N	VAL	F	75	66.955	67.215	72.629	1.00	46.10	F
ATOM	9428	CA	VAL	F	75	68.160	67.954	72.299	1.00	47.48	F
ATOM	9429	CB	VAL	F	75	68.310	68.207	70.759	1.00	48.87	F
ATOM	9430	CG1	VAL	F	75	67.087	68.967	70.200	1.00	41.65	F
ATOM	9431	CG2	VAL	F	75	69.599	68.971	70.498	1.00	38.69	F
ATOM	9432	C	VAL	F	75	68.057	69.282	73.031	1.00	46.89	F
ATOM	9433	O	VAL	F	75	67.070	70.015	72.881	1.00	41.30	F
ATOM	9434	N	LYS	F	76	69.060	69.567	73.852	1.00	47.29	F
ATOM	9435	CA	LYS	F	76	69.077	70.820	74.581	1.00	50.34	F
ATOM	9436	CB	LYS	F	76	69.597	70.621	76.009	1.00	51.71	F
ATOM	9437	CG	LYS	F	76	69.270	71.788	76.933	1.00	55.24	F
ATOM	9438	CD	LYS	F	76	69.735	71.555	78.363	1.00	60.80	F
ATOM	9439	CE	LYS	F	76	69.274	72.695	79.284	1.00	63.97	F
ATOM	9440	NZ	LYS	F	76	69.701	72.497	80.706	1.00	68.67	F
ATOM	9441	C	LYS	F	76	69.973	71.813	73.843	1.00	51.42	F
ATOM	9442	O	LYS	F	76	71.199	71.697	73.870	1.00	50.94	F
ATOM	9443	N	TYR	F	77	69.348	72.785	73.183	1.00	49.81	F
ATOM	9444	CA	TYR	F	77	70.084	73.805	72.456	1.00	49.19	F
ATOM	9445	CB	TYR	F	77	69.556	73.963	71.036	1.00	40.66	F
ATOM	9446	CG	TYR	F	77	70.390	74.929	70.234	1.00	42.35	F
ATOM	9447	CD1	TYR	F	77	71.763	74.744	70.107	1.00	40.77	F
ATOM	9448	CE1	TYR	F	77	72.530	75.592	69.330	1.00	44.94	F
ATOM	9449	CD2	TYR	F	77	69.808	76.004	69.566	1.00	45.11	F
ATOM	9450	CE2	TYR	F	77	70.567	76.867	68.778	1.00	38.35	F
ATOM	9451	CZ	TYR	F	77	71.931	76.652	68.658	1.00	46.15	F
ATOM	9452	OH	TYR	F	77	72.700	77.449	67.825	1.00	47.81	F
ATOM	9453	C	TYR	F	77	70.032	75.180	73.099	1.00	52.24	F
ATOM	9454	O	TYR	F	77	69.024	75.880	72.973	1.00	54.64	F
ATOM	9455	N	SER	F	78	71.111	75.575	73.765	1.00	51.37	F
ATOM	9456	CA	SER	F	78	71.167	76.901	74.361	1.00	52.39	F
ATOM	9457	CB	SER	F	78	71.001	77.961	73.249	1.00	51.04	F
ATOM	9458	OG	SER	F	78	71.215	79.296	73.699	1.00	46.53	F
ATOM	9459	C	SER	F	78	70.098	77.095	75.429	1.00	55.65	F
ATOM	9460	O	SER	F	78	69.308	78.036	75.361	1.00	58.01	F
ATOM	9461	N	GLY	F	79	70.055	76.204	76.410	1.00	58.16	F
ATOM	9462	CA	GLY	F	79	69.067	76.364	77.463	1.00	62.32	F
ATOM	9463	C	GLY	F	79	67.700	75.728	77.271	1.00	63.66	F



ATOM	9464	O	GLY	F	79	67.064	75.372	78.257	1.00	65.24	F
ATOM	9465	N	SER	F	80	67.239	75.594	76.027	1.00	63.68	F
ATOM	9466	CA	SER	F	80	65.935	74.984	75.749	1.00	63.15	F
ATOM	9467	CB	SER	F	80	65.156	75.841	74.762	1.00	60.98	F
ATOM	9468	OG	SER	F	80	64.840	77.081	75.354	1.00	68.24	F
ATOM	9469	C	SER	F	80	66.041	73.558	75.203	1.00	63.15	F
ATOM	9470	O	SER	F	80	67.094	73.156	74.697	1.00	62.36	F
ATOM	9471	N	SER	F	81	64.949	72.796	75.302	1.00	60.19	F
ATOM	9472	CA	SER	F	81	64.947	71.417	74.817	1.00	54.17	F
ATOM	9473	CB	SER	F	81	64.682	70.428	75.958	1.00	56.00	F
ATOM	9474	OG	SER	F	81	65.892	69.881	76.466	1.00	55.39	F
ATOM	9475	C	SER	F	81	63.950	71.187	73.706	1.00	50.61	F
ATOM	9476	O	SER	F	81	62.938	71.860	73.601	1.00	47.11	F
ATOM	9477	N	TYR	F	82	64.264	70.231	72.850	1.00	52.61	F
ATOM	9478	CA	TYR	F	82	63.400	69.919	71.728	1.00	51.05	F
ATOM	9479	CB	TYR	F	82	63.838	70.695	70.469	1.00	52.08	F
ATOM	9480	CG	TYR	F	82	64.098	72.175	70.692	1.00	54.57	F
ATOM	9481	CD1	TYR	F	82	65.221	72.610	71.399	1.00	51.96	F
ATOM	9482	CE1	TYR	F	82	65.431	73.967	71.666	1.00	55.73	F
ATOM	9483	CD2	TYR	F	82	63.192	73.140	70.243	1.00	59.64	F
ATOM	9484	CE2	TYR	F	82	63.393	74.508	70.501	1.00	55.89	F
ATOM	9485	CZ	TYR	F	82	64.513	74.912	71.214	1.00	59.54	F
ATOM	9486	OH	TYR	F	82	64.713	76.254	71.480	1.00	63.13	F
ATOM	9487	C	TYR	F	82	63.489	68.423	71.461	1.00	48.76	F
ATOM	9488	O	TYR	F	82	64.437	67.741	71.878	1.00	49.60	F
ATOM	9489	N	PRO	F	83	62.499	67.894	70.755	1.00	43.46	F
ATOM	9490	CD	PRO	F	83	61.289	68.612	70.346	1.00	40.53	F
ATOM	9491	CA	PRO	F	83	62.415	66.480	70.400	1.00	44.18	F
ATOM	9492	CB	PRO	F	83	61.075	66.388	69.691	1.00	42.13	F
ATOM	9493	CG	PRO	F	83	60.296	67.514	70.289	1.00	44.41	F
ATOM	9494	C	PRO	F	83	63.557	66.061	69.486	1.00	45.02	F
ATOM	9495	O	PRO	F	83	63.829	66.726	68.484	1.00	47.21	F
ATOM	9496	N	PHE	F	84	64.224	64.960	69.815	1.00	45.86	F
ATOM	9497	CA	PHE	F	84	65.326	64.466	68.977	1.00	44.64	F
ATOM	9498	CB	PHE	F	84	66.660	64.592	69.704	1.00	44.94	F
ATOM	9499	CG	PHE	F	84	67.822	64.033	68.935	1.00	42.64	F
ATOM	9500	CD1	PHE	F	84	68.389	64.749	67.888	1.00	40.91	F
ATOM	9501	CD2	PHE	F	84	68.337	62.770	69.239	1.00	39.71	F
ATOM	9502	CE1	PHE	F	84	69.454	64.213	67.155	1.00	40.95	F
ATOM	9503	CE2	PHE	F	84	69.401	62.232	68.508	1.00	38.02	F
ATOM	9504	CZ	PHE	F	84	69.959	62.958	67.466	1.00	34.23	F
ATOM	9505	C	PHE	F	84	65.062	62.996	68.656	1.00	45.21	F
ATOM	9506	O	PHE	F	84	64.875	62.177	69.567	1.00	48.91	F
ATOM	9507	N	PRO	F	85	65.090	62.624	67.363	1.00	44.00	F
ATOM	9508	CD	PRO	F	85	64.852	61.212	67.011	1.00	39.93	F
ATOM	9509	CA	PRO	F	85	65.319	63.415	66.146	1.00	43.11	F
ATOM	9510	CB	PRO	F	85	64.855	62.475	65.044	1.00	39.52	F
ATOM	9511	CG	PRO	F	85	65.324	61.149	65.569	1.00	37.09	F
ATOM	9512	C	PRO	F	85	64.560	64.721	66.168	1.00	42.70	F
ATOM	9513	O	PRO	F	85	63.465	64.777	66.710	1.00	45.67	F
ATOM	9514	N	THR	F	86	65.135	65.769	65.591	1.00	40.24	F
ATOM	9515	CA	THR	F	86	64.482	67.065	65.601	1.00	40.17	F
ATOM	9516	CB	THR	F	86	65.469	68.168	65.273	1.00	37.73	F
ATOM	9517	OG1	THR	F	86	65.892	68.032	63.913	1.00	34.54	F
ATOM	9518	CG2	THR	F	86	66.672	68.100	66.193	1.00	38.84	F
ATOM	9519	C	THR	F	86	63.347	67.120	64.605	1.00	44.75	F
ATOM	9520	O	THR	F	86	63.294	66.317	63.677	1.00	45.99	F
ATOM	9521	N	THR	F	87	62.446	68.078	64.796	1.00	48.99	F



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